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INTRODUCTION

The Institute for Computer Applications in Science and Engineering (ICASE) is operated at the Langley Research Center (LaRC) of NASA by the Universities Space Research Association (USRA) under a contract with the Center. USRA is a nonprofit consortium of major U. S. colleges and universities.

The Institute conducts unclassified basic research in applied mathematics, numerical analysis, and computer science in order to extend and improve problem-solving capabilities in science and engineering, particularly in aeronautics and space.

ICASE has a small permanent staff. Research is conducted primarily by visiting scientists from universities and from industry, who have resident appointments for limited periods of time, and by consultants. Members of NASA's research staff also may be residents at ICASE for limited periods.

The major categories of the current ICASE research program are:

- Numerical methods, with particular emphasis on the development and analysis of basic numerical algorithms;
- Control and parameter identification problems, with emphasis on effective numerical methods;
- Computational problems in engineering and the physical sciences, particularly fluid dynamics, acoustics, and structural analysis;
- Computer systems and software for parallel computers.

ICASE reports are considered to be primarily preprints of manuscripts that have been submitted to appropriate research journals or that are to appear in conference proceedings. A list of these reports for the period April 1, 1991 through September 30, 1991 is given in the Reports and Abstracts section which follows a brief description of the research in progress.

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RESEARCH IN PROGRESS

Saul Abarbanel

The study of the stability of hyperbolic initial-boundary value problems has led to an ICASE Report by Carpenter, Gottlieb and Abarbanel entitled: "The Stability of Numerical Boundary Treatments for Compact High Order Finite Difference Schemes".

The above study relied heavily on numerical evaluations of various stability criteria. Together with David Gottlieb, additional theoretical studies were carried out to discover under which norms one might be able to prove stability. For 1st and 2nd order numerical boundary conditions this issue has been resolved and stability proved. This work now continues with regard to higher order boundary conditions and for the more general case of systems.

The work (together with doctoral student J. Danowitz) on non-reflecting boundary conditions for compressible viscous flow past two-dimensional finite bodies continues.

Remi Abgrall

We have tried to design an Essentially Non Oscillatory reconstruction for functions defined on finite-element type meshes. Two related problems are studied : the interpolation of possibly unsmooth multivariate functions on arbitrary meshes and the reconstruction of a function from its average in control volumes surrounding the nodes of the mesh. Concerning the first problem, we have studied the behavior of the highest coefficients of the Lagrange interpolation functions which may admit discontinuities of locally regular curves. This enables us to choose the best stencil for its interpolation. The choice of the smallest possible number of stencils is addressed. Concerning the reconstruction problem, because of the very nature of the mesh, the only method that may work is the so called reconstruction via deconvolution method. Unfortunately, it is well suited only for regular meshes as we show, but we also show how to overcome this difficulty. The global method has the expected order of accuracy but is conservative up to a high order quadrature formula only.

Some numerical examples which demonstrate the efficiency of the method are given in a forthcoming ICASE report.

H. T. Banks and Fumio Kojima

Work is continuing on the study of the corrosion detection problem arising in thermal tomography. In conjunction with W.P. Winfree (Nondestructive Evaluation Sciences Branch, LaRC), we have developed practical corrosion detection algorithms based on nonlinear least

square estimation. Computational efficiency is a very important factor in implementing nondestructive evaluation techniques. The latest version of our algorithm is at least four times faster than the earlier one. The choice of the regularization parameter in our geometrical heat inverse problem has been studied also. A graphical method to find the optimal choice of the regularized parameters has been investigated; this method involves plotting the seminorm of the solution versus the residual norm.

H. T. Banks and Ralph Smith

Work is continuing on the development of a computationally viable infinite-dimensional control and identification methodology for the stable and optimal design of noise suppression systems. The basic approach is to combine approximation theory with time domain state space modeling to develop convergent computational algorithms for LQR control designs.

The model to be considered consists of an exterior noise source which is separated from an interior chamber by an active wall or plate. This plate transmits noise or vibrations from the exterior field to the interior cavity via fluid/structure interactions thus leading to the formulation of a system of partial differential equations consisting of a 3-D acoustic wave equation coupled with elasticity equations for the plate. The control is implemented in the model via piezoceramic patches on the plate which are excited in a manner so as to produce pure bending moments. The validity of the model is being tested both numerically and with data from experiments by H.C. Lester and R.J. Silcox (Acoustics Division, LaRC).

As an initial test of the control methodology, a simplified but typical model consisting of a 2-D interior cavity with an active beam at one end has been considered. We have found that a Legendre basis in the cavity coupled with a cubic spline discretization of the beam provides a scheme which efficiently handles the numerical difficulties resulting from the lack of a uniform margin of stability and the fact that the system is only weakly damped. Numerical tests have shown that when the feedback controls are implemented, substantial reductions in acoustic pressure can be realized with physically realistic voltages into the patches. Further numerical tests are being made to determine optimal patch placements, numbers and lengths for the 2-D model.

Current and future work is also being directed toward developing an accurate, efficient and stable means of discretizing the 3-D model in which the interior cavity is taken to be cylinder with a circular active plate and sectorial patches. Once the 3-D approximation scheme has been completed, the identification of physical parameters and control of acoustic pressure will be implemented using techniques similar to those developed for the 2-D problem.

Alvin Bayliss

In collaboration with L. Maestrello (Fluid Mechanics Division, LaRC) and A. Frendi (Vigyan, Inc.), we consider the evolution of unsteady disturbances in a supersonic boundary layer over a flexible surface. The problem is solved numerically. The unsteady flow field disturbances are computed by direct solution of the Navier-Stokes equations. The motion of the wall is computed by solution of the equations governing a flexible surface clamped at each end. These equations are coupled, as the plate equation is forced by the pressure computed from the Navier-Stokes equations which in turn requires the solution of the plate equation as a boundary condition.

We consider the case where the plate is forced by an instability wave in the flow field as well as the case where the flexible source is excited by an acoustic disturbance. Results obtained to date demonstrate that the growth of disturbances can be enhanced when the bounding surface is flexible.

H. Scott Berryman

In cooperation with Intel Scientific Supercomputing Division, and with the collaboration of W. Gropp (Argonne National Laboratory) and R. Littlefield (Pacific Northwest Laboratory) the behavior of the Touchstone DELTA system interprocessor communication subsystem has been studied. The goal is to gather data to aid in protocol development, application optimization and the development of interprocessor global operations such as the global reduction, and global transpose.

In collaboration with S. Bokhari algorithms for the global transpose for two dimensional grids in general, and the DELTA system in particular, are being studied. The global transpose is needed in such scientific codes as multidimensional FFTs, unstructured mesh codes (for address translation using lookup tables) and ADI methods.

Nicholas Blackaby

Work on the stability of hypersonic flow over a flat plate in collaboration with S. Cowley (Cambridge University) and P. Hall was completed. A paper based on an earlier ICASE report by the authors has been submitted to the Journal of Fluid Mechanics.

Research into vortex-wave interactions in compressible boundary layer flows has continued. The weakly non-linear interaction of Tollmien-Schlichting waves and longitudinal vortices has been considered, in collaboration with F.T. Smith (UC London). The inviscid stability of a small-wavelength, fully nonlinear Gortler vortex state in a large-Mach number Blasius boundary layer was investigated during the LaRC/ICASE Transition and Turbulence

workshop; a report on this work has been submitted to the workshop proceedings.

Together with M. Choudhari (High Tech. Inc.), the nonlinear development of longitudinal vortices in the presence of wall-curvature and cross-flow is presently being considered. In most practical aerodynamic applications there will be a significant amount of cross-flow normal to the principal direction of flow. Cross-flow has previously been shown to have a dramatic effect on the linear stability properties of Gortler vortices. We have found that, above a certain size of cross-flow, neutrally stable longitudinal vortices are possible over a convex surface. We are currently investigating the weakly nonlinear development of these modes (for both concave and convex wall curvatures). The problem is mathematically very similar to studies into the stability of stratified flows in geophysical applications. Thus we are able to apply some of the methods of the latter to our study. A Landau amplitude equation will be derived from which nonlinear development properties can be deduced. An ICASE report describing this work should follow early in 1992.

Percy Bobbitt

A paper concerning the background of, and results from, the hybrid laminar flow control (HLFC) experiment carried out in the LaRC's 8-ft Transonic Preserve Tunnel on a swept, 7-foot chord model has been written and is awaiting final review and publication. A shortened version of this paper has also been prepared for presentation at the Annual AIAA Conference in Reno, Nevada and is now being reviewed. Both papers discuss the design of the HLFC airfoil's upper-surface contour and the associated pressure distribution. Results for variations in Mach number, Reynolds number, level and extent of suction are illustrated and analyzed. The results are given primarily as plots of transition location, suction mass-flow requirements, pressure distribution and drag.

Shahid Bokhari

A major overhead in interprocessor communications on distributed memory machines is the time required to permute data blocks when using a 'combining' algorithm. The time required to shuffle blocks in the 'standard exchange' algorithm for complete exchange on hypercubes is an important (though not the only) example. I am developing an enhanced DMA unit that will eliminate the overhead of this data permutation at the cost of a modest investment in hardware. Since this overhead can be as much as 50% of the total communication time, this enhancement is likely to be of considerable practical value.

A theoretical analysis of the multiphase algorithm for complete exchanges on the hypercube is also underway. In this case I am attempting to develop a method for efficiently obtaining the optimal algorithm, given a specific block size and hypercube dimension.

Shahid Bokhari and Scott Berryman

Work is underway on developing a class of algorithms for complete exchange on the Touchstone Delta Mesh. The complete exchange is at the heart of many important applications. The mesh interconnect is much sparser than the hypercube and there is no possibility of an asymptotically optimal 'direct' algorithm, as was the case for hypercubes. We are developing a multiphase combining algorithm which trades off the startups of the direct algorithm with the overhead of data permutation. A theoretical analysis is nearly complete and we are in the process of obtaining actual run times on the Touchstone Delta machine.

Kurt Bryan

Work is continuing with W.P. Winfree (Nondestructive Evaluative Sciences Branch, LaRC) on a thermo-mechanical inverse problem, specifically, using the surface mechanical response of a structure to external heating to determine its internal properties and/or locate defects. The focus is on structures which are thermally and mechanically isotropic and homogeneous. Analysis of the forward problem leads to a system of partial differential equations, the heat equations coupled to the equations of linear elasticity. Due to the complicated nature of the equations, the computational solution of the inverse problem will probably rely on an optimization/fit-to-data approach. This requires an economical scheme for solving the forward problem. A program has been written to solve the forward problem, based on the method of boundary integral equations. This approach should be particularly efficient, since the inverse problem requires the mechanical response of the structure only on its surface. We are now pursuing appropriate convergence results for the numerical method and a sensitivity analysis to determine the optimal experimental configuration for locating internal defects.

Work is also underway with M. Vogelius (Rutgers University) on a version of the inverse conductivity problem. The goal is to recover information about multiple internal cracks in an electrical conductor based on voltage and current flux measurements on its boundary. Theoretical results concerning the detection and identification of multiple internal cracks in a conductor have been proved. A numerical algorithm is also under development, based on

an integral equation formulation of the problem. This formulation and code should lead to results for the optimal electrode arrangement and computational solution of the inverse problem.

Thomas W. Crockett

The iPSC/860 version of the parallel renderer was modified to generate sequences of images using both temporal and spatial compression. This is an attractive technique for producing live animation on the iPSC/860 given the low bandwidth of its external connections. A companion interpreter for the compressed image format was developed which uses the X Window System and Unix sockets to display the output remotely on users' workstations. The interpreter will also run directly on the iPSC/860 to play back previously recorded sequences stored on the Concurrent File System. The combination of the renderer and interpreter serves as the first demonstration at Langley of the iPSC/860's backend CIO Ethernet interface. The techniques employed have wide applicability in other distributed codes which are being developed for the machine.

A new release of the iPSC/860 system software from Intel was installed. The new software, while providing critically needed functionality, proved to be less stable than the previous version, resulting in a series of system crashes with major filesystem damage. Consequently, disk backup and restore procedures were refined so that recovery time could be reduced from 14 hours to 5 hours. Pressure from ICASE and other sites has convinced Intel to provide monthly software updates.

Intel's system software currently provides little assistance in sharing resources fairly among users. With our relatively large user community, this was becoming a serious problem. After investigating several alternatives, we were able to acquire a job scheduling package under development at the San Diego Supercomputer Center. We are currently acting as a beta site for this software, which we expect to be incorporated into a future release from Intel. The SDSC software has been very successful, virtually eliminating the resource management problem.

Wai-Sun Don

In collaboration with A. Solomonoff, the research about the accuracy and speed in computing the Chebyshev collocation derivative was completed, and a paper describing the results was submitted to the SIAM Journal on Scientific and Statistical Computing for publication.

Collaborating with P. Drummond (Fluid Mechanics Division, LaRC), a three dimensional

spectral code for solving the hydrogen vortex jet interaction with an oblique shock using Chebyshev collocation methods is currently under development. The preliminary results of the air vortex jet interaction with an oblique shock look quite promising. Chemical reactions with different species will also be included in the calculation to simulate the physics in the scramjet engine.

Peter W. Duck

The interaction between a shock wave and various forms of freestream disturbance (i.e. vorticity waves, entropy waves and acoustic waves) is currently under investigation. On passing through the shock, any one of these waves will, in general, generate all three classes of wave. The specific configuration under study involves a wedge (which is responsible for the creation of the shock), and the effect of disturbances ahead of the shock on the boundary layer on the wedge surface is of particular interest. There are a number of other issues related to this problem currently under study, including the effect of wedge surface distortion, and the possibility of altering the shock strength.

Thomas Eidson

An explicit, finite-difference code developed by G. Erlebacher to study 3-D, compressible turbulence was converted to the Intel iPSC/860 to evaluate various performance programming ideas. Two versions which have different distribution strategies have been implemented. One version uses across-processor transposes to get the appropriate data on each processor to perform the tridiagonal matrix solutions. The second version solves the tridiagonal matrix problem with an algorithm that works with the appropriate data distributed across several processors. Both versions attain between 5 and 8 Mflops per node. Problem sizes up to 64x64x64 have been tested. Larger sizes will be tested when the initial condition code is running on the hypercube. More extensive data analysis, which includes an FFT algorithm, is also being implemented. This code has also been used to study several problems in programming in a multi-machine environment. The code was modified so that minimum differences exist between the CRAY version and the hypercube version. The code was also modified to run different segments of the code on different computers: the control segment runs on a workstation, the main calculations run on the hypercube and the monitor/graphics segments runs on a graphics workstation.

A vector library (written in assembler) was written and tested. There does not appear to be any significant benefit of using a vector library over the compiler in the general case. This is partially due to significant improvements in the compiler. For code sections for which

the data could reside in cache and be reused, assembler coding may provide some benefit. An example would be an FFT.

A project to develop a code transformation tool was begun. With an increasing number of computers with varying architectures becoming available, moving codes between computers is being done more frequently even though it is becoming more difficult. The design of new compilers and automatic pre-processors is not keeping up with the demand. The transformation tool is designed to aid the user in porting codes by handling the details of the code changes with fewer errors, thus reducing the debugging effort. The user will be required to determine the appropriate transformations and thus do the appropriate data dependency or data flow analysis. This strategy will hopefully provide a useful porting tool more quickly than developing a compiler or pre-processor that does most of the code analysis.

Gordon Erlebacher

Current collaboration with S. Sarkar is focused on the analysis of compressible shear turbulent flow databases that he generated in the last year. The objective is to elucidate the effect of compressibility on the well-known structures of incompressible shear-flow turbulence. The results of this work will be submitted to Physics of Fluids and presented at the APS meeting.

First hand knowledge of wavelet theory and its potential applications to CFD was obtained at a meeting on wavelets at Princeton University. This led to a collaboration with C. Streett (Fluid Mechanics Division, LaRC), in which several diagnostics were developed based wavelet transforms to perform a quantitative study of long time signals obtained from the direct simulation of finite-length incompressible Taylor Couette flow. This allowed the frequency content of the signal to be analyzed as a function of time. The results of this work were presented at the International Fluids conference in Nobeyama, Japan. A report will be written and submitted to the conference proceedings.

Work is still in progress with S. Biringen and F. Hatay (Colorado State University) on the direct numerical simulation of compressible Couette flow. During the transition workshop, Hatay and I checked the linear stability theory, and he has gone on to do the nonlinear calculations.

James F. Geer

Work is continuing on hybrid perturbation/variational techniques for solving systems of either ordinary or partial differential equations. For ODE's, we are currently applying the methods to several classes of nonlinear vibration problems, with special emphasis on resonant

frequency calculations for systems of equations written in Lagrangian or Hamiltonian form. For PDE's, we are investigating how the method might be applied to some exterior boundary value problems for elliptic PDE's, when the boundary of the domain D has an irregular shape. The basic idea is to treat D as a perturbation of a simple domain R (e.g. a circle or an ellipse, in two dimensions) by embedding it in a one parameter family of domains indexed by a parameter a , where $0 \leq a \leq 1$. Currently, we are applying the method to some eigenvalue problems for irregularly shaped domains and to some problems of flows about geometrically complicated bodies. In addition, we are combining our method with some homotopy methods to further enhance the accuracy of the results we obtain. In particular, we hope this will lead to a new extension of slender body theory. So far, the preliminary results have been encouraging. Work on the method itself is being done with C. Andersen (College of William and Mary), while possible applications are being discussed with E. Liu (Fluid Mechanics Division, LaRC).

The problem of describing aerodynamically generated sound from compact sources of vorticity is being studied from a perturbation point of view, with the eddy Mach number appearing as the perturbation parameter. The problem appears to be well suited to an application of a slightly modified version of the method of multiple scales. In particular, the problem of determining the sound generated by a sphere executing arbitrary (small) oscillations in zero mean flow conditions has been investigated successfully by this technique. Once the perturbation solution is fully understood, the hybrid perturbation Galerkin technique will be applied to it, with the goal of extending the usefulness (and accuracy) of the solution to higher Mach numbers than is possible using the perturbation solution alone. This work is being carried out with J. Hardin (Acoustics Division, LaRC).

David Gottlieb

We have continued our work on the asymptotic stability of high order finite difference schemes. In an ICASE report (together with Abarbanel and Carpenter) we reported the new phenomenon that high order schemes tend to allow solutions that grow in time. The reason is that the *inflow* boundary conditions are more involved. We try to solve this problem in several ways. The first approach is to use penalty type boundary conditions to control this growth in time. Using this approach we are testing now a compact fourth order scheme with penalty boundary conditions that seems to be asymptotically stable even for systems of equations. The second approach is to construct boundary conditions in such a way that the scheme satisfies the same energy estimate as the differential equation itself. In joint work with Gustafsson we showed that it can be done for explicit schemes but not for compact schemes. We feel that the problem has to be answered before compact schemes can be used

for problems involving long time integration.

We have solved the classical problem of the Gibbs phenomenon. It is well known that if we are given the first N Fourier modes of an analytic *and periodic function* then the Fourier approximation, based on modes converges exponentially. Gibbs (in 1898) showed that if the function is not periodic, then the rate of convergence is $\frac{1}{N}$ away from the discontinuity and there is a constant overshoot in the neighborhood of the discontinuity (in this case the boundary).

We have shown that one could construct, with exponential accuracy, the coefficients of the expansion of the function based on the Gegenbauer polynomials $c_{\frac{N}{3}}^{\frac{N}{3}}$. Thus we can recover the exponential accuracy up to and including the discontinuities.

Ami Harten

In collaboration with S. R. Chakravarthy (Rockwell International Science Center) we have developed a class of ENO schemes for the numerical solution of multidimensional hyperbolic systems of conservation laws in structured and unstructured grids. This is a class of shock-capturing schemes which is designed to compute cell-averages to high-order accuracy. The ENO scheme is composed of a piecewise-polynomial reconstruction of the solution from its given cell-averages, approximate evolution of the resulting initial-value problem, and averaging of this approximate solution over each cell. The reconstruction algorithm is based on an adaptive selection of the stencil for each cell so as to avoid spurious oscillations near discontinuities while achieving high order accuracy away from them.

I have begun to work on multi-resolution analysis for ENO schemes. Given a function $u(x)$ which is represented by its cell-averages in cells which are formed by some unstructured grid, we decompose the function into various scales of variation. This is done by considering a set of nested grids in which the given grid is the finest, and identifying in each locality the coarsest grid in the set from which $u(x)$ can be recovered to a prescribed accuracy.

Multi-resolution analysis is applied to ENO schemes in order to reduce the number of numerical flux computations which is needed in order to advance the solution by one time-step. This is accomplished by decomposing the numerical solution at the beginning of each time-step into levels of resolution, and performing the computation in each locality at the appropriate coarser grid. We are studying an efficient algorithm for implementing this concept in the one-dimensional case; this algorithm can and will be extended to the multi-dimensional case with cartesian grids.

Thomas L. Jackson

Work focuses on the time evolution of the interaction of a diffusion flame with a vortex in a weak acoustic field, directly applicable to the large scale structures found in compressible mixing layers. In particular, the ignition process is under current investigation. In addition, the effects of compressibility will be studied. A combination of asymptotics and numerics will be used to reduce the complex problem to a model problem, thus isolating key physical effects for analysis. This work is in collaboration with M. Macaraeg (Fluid Mechanics Division, LaRC) and M.Y. Hussaini.

Peter A. Jacobs

A single-block Navier-Stokes solver was completed and was documented in Interim Report 18 and Report 91-75. The code was then applied to the simulation of transient flow in a reflected-shock tunnel with a large Mach number nozzle and results were reported in Report 91-60. An interesting feature found in the simulation was the formation of a vortex near the tube centreline just upstream of the nozzle throat. Theoretical models presently used for the prediction of test-gas contamination in reflected-shock tunnels may need to be modified to include the effects of the vortex. However, further work is required to determine sensitivity of the simulations to grid distortions and facility operating conditions.

The code was also used to simulate the operation of the Langley expansion tube with helium as the working gas. Preliminary results were reported in Interim Report 20. The agreement between experimental measurements and the simulation results indicates that we now have a reliable tool which may be used to study some of the multidimensional flow processes in expansion tubes. An understanding of these processes is key to improving the quality of the test flow produced. Since each simulation required some 50 hours of CPU time on a Cray-Y/MP and most of the parameter space has yet to be explored, we may attempt a parallel implementation of the code in the near future.

Ashwani Kapila

Under appropriate conditions, a compressive pulse propagating through an exothermically reacting atmosphere steepens and amplifies, eventually resulting in a local thermal runaway and a shock. In collaboration with T. Jackson, I have been studying the post-runaway evolution of the pulse. Of special interest is the case when the runaway occurs on the shock itself. Our analysis is asymptotic, and is a portion of a continuing project on the transient events that occur prior to the establishment of detonation waves.

David E. Keyes

The divide-and-conquer paradigm of iterative domain decomposition, or substructuring, has become a practical tool in computational fluid dynamics applications because of its flexibility in accommodating adaptive refinement through locally quasi-uniform grids, its ability to exploit multiple discretizations of the operator equations, and the modular pathway it provides towards parallelism. Two-scale domain-decomposed preconditionings consisting of a coarse grid of subdomain vertices and a large number of independent subdomain problems are strong enough to provide convergence rates within a log-factor of optimal as the grid is refined, without requiring data exchanges between subdomains on a full hierarchy of scales at each iteration. Thus, such algorithms are promising for loosely coupled distributed memory computers with high communication latency, including workstation networks.

Recently we have been seeking generalizations of the diffusively-dominated work described in earlier ICASE Reports 91-19 and 91-20 to high Reynolds number conditions and indefinite (Helmholtz) problems.

Marten T. Landahl

Work has primarily been directed at analysing the role of algebraic instability on streak formation and flow structure in the near-wall region of a turbulent boundary layer. To this purpose I have looked at the space-time evolution of a localized three-dimensional disturbance in a strong shear flow, paying particular attention to viscous and nonlinear effects.

D. Glenn Lasseigne

New research involves the response of a boundary layer behind a nonreacting shock wave supported by a wedge. Disturbances are produced as the wedge shape changes or as vorticity disturbances in the mean field are propagated through the shock.

Continuing research focuses on the interactions of disturbances in the flow field with both reacting and non-reacting shocks. A combination of asymptotics and numerics is used to reduce complex problems to model problems, thus isolating key physical effects for analysis. Specific problems include: the non-linear interactions of vorticity/detonation waves, the effects of heat release on the response of an oblique detonation subjected to wedge oscillations, and the coupling of upstream disturbances and wedge oscillations on the stability of an oblique detonation. The goal is to develop numerical routines which capture the instability modes predicted by linear theory. Other problems include the effects of streamwise vorticity on the stagnation point flow and the effects of more general disturbances on a flame in the viscous stagnation region.

Dimitri Mavriplis

Work is continuing on the use of unstructured meshes for solving computational fluid dynamics problems in both two and three dimensions.

In two dimensions, an implicit solver for the full Navier Stokes equations on unstructured meshes has been developed in conjunction with V. Venkatakrishnan (Computer Science Corporation). The method consists of an ILU (incomplete LU factorization) preconditioned GMRES implicit iterative technique. In a recent paper (ICASE Report 91-40) this strategy was found to provide superior efficiency compared to other preconditioners and other implicit iteration techniques, while approaching the computational efficiency of previously developed unstructured multigrid techniques.

In three dimensions, an inviscid flow solver has been developed incorporating adaptive meshing techniques and an unstructured multigrid algorithm, thus enabling the efficient and accurate computation of three-dimensional flow fields about complex configurations (ICASE Report 91-40). Work is continuing on the demonstration of the efficiency of this technique with the application of a large scale computation about a complete aircraft configuration using a fine mesh of over 0.6 million points.

Future work will be directed at evaluating new turbulence models for the two-dimensional problems. In three dimensions, the investigation of new more efficient and robust gridding and adaptive mesh refinement techniques will be pursued.

In conjunction with J. Saltz, Subhendu Das, and Ravi Ponnusamy, the three-dimensional unstructured multigrid Euler solver (non-adaptive) has been implemented on the Intel Hypercube using the PARTI primitives. This work is aimed at demonstrating the applicability of the PARTI primitives to practical implementations, and also to employ experience gained from particular implementations to aid in the design or modification of the primitives. A large scale computation over a complete aircraft configuration running on the iPSC 860 is in the planning stages in order to demonstrate the efficiency of the parallelized code. The implementation will be extended in the future to include the use of adaptive meshing strategies.

Piyush Mehrotra

Current research in languages and compilers for distributed memory machines has focussed on exclusively exploiting data parallelism present in algorithms. However, in addition to this loop level parallelism, scientific applications also exhibit functional parallelism at a coarser level. We have been investigating an integrated approach which allows the user to efficiently exploit both levels of parallelism on distributed memory architectures. In pursuing this approach, several issues need to be resolved both at the user (source) level and also at

the system/runtime level.

At the language level, we need to define models/constructs which allow the user to specify both the coarse grain and the fine grain parallelism so that the two do not conflict with each other. The main objective here is to provide minimal extensions to FORTRAN which strike a balance between allowing the user to control factors which critically affect performance and hiding the low level details which can be automatically handled by the compiler/runtime system. At the system level the most critical issue is the management of resources such as processors and memory. In the above model, we have loosely synchronous groups of processes interacting asynchronously with other such groups. Each group of processes needs to be scheduled across a set of processors simultaneously both from the point of avoiding deadlock and also from the point of efficiency. Messages between such groups involve distributed data; thus massaging from one distribution to another before the messages are delivered may be required.

The overall objective of the project is to provide a system which allows all levels of parallelism in a scientific application to be efficiently mapped onto distributed memory machines.

In joint effort with K.-Y. Wang (Purdue University), we have been investigating an optimization technique called message consolidation which attempts to reduce the communication and synchronization cost by decreasing the number of messages sent through the communication network. However, in certain situations, such combining of messages may increase the data synchronization delays thus leading to poorer overall performance. We have designed an algorithm for message consolidation and have been investigating heuristics for recognizing situations where such a transformation can be profitably applied.

H. S. Mukunda

An opposed jet diffusion flame (OJDF) model with finite rate chemistry is being used to explain the weak thermal development of a reacting high speed hydrogen-air mixing layer which shows small departure of the reaction rates from equilibrium. The use of modified flame surface theory permits the reduction to the solution of a set of algebraic equations involving chemistry of seven species and nine reversible reactions. The use of this simple theory is justified by noting that numerical calculations with full chemistry show a single sharp flame front. The solution of the equations is first compared with recent data on hydrogen-air OJDF obtained at LaRC. The stretch parameters are extracted from the direct numerical simulations of the reacting mixing layer with full chemistry. The results of OJDF for these parameters clearly indicate that even though peak temperatures and species mass

fractions depart from adiabatic values very significantly, the departures of the reaction rates from equilibrium are not large. The effects of Lewis numbers on the flame behavior at high temperatures are extracted from the calculations.

Naomi Naik and John Van Rosendale

We are concentrating on understanding boundary layer issues in Navier Stokes codes. We analyzed and experimentally tested various multiple semi-coarse grid methods, both sequential and parallel versions, for their suitability for thin cells and stretched grids. We are also completing some past work on spectral preconditioning and determining the complexity of concurrent multigrid which will appear as ICASE reports.

Work on robust parallel multigrid algorithms is continuing in collaboration with J. Dendy (Los Alamos National Laboratory). As is well known, to achieve fast convergence on general tensor product grids, multigrid algorithms based on line or plane relaxation must be used. In three dimensions, only plane-relaxation suffices, in general. Unfortunately, plane relaxation multigrid is very difficult to parallelize effectively. Several groups have designed experimental parallel implementations of such algorithms, with mixed results.

A better alternative for achieving robust parallel elliptic solvers is to use multiple coarse grids, formed by semi-coarsening the grid separately in each of the coordinate directions, together with a simple point-relaxation smoother. This idea, closely related to the hyperbolic algorithm of W. Mulder, can be used to create robust and effective elliptic solvers. A class of such algorithms now exists, differing mainly in the ways the separate coarse grid solutions are combined.

In recent work, we have established the rapid convergence of the first of these algorithms, in which the solutions from separate coarse grids are combined via a local "switch," based on the strength of the discrete operator in each coordinate direction. An improved version of this algorithm now exists, free of the necessity of computing the local switch, but we have not yet established its rapid convergence.

In related work, we are developing a variant of this algorithm for problems having severe coefficient jumps and strong grid stretching. By combining the new algorithm with interpolation formulas developed previously for plane relaxation algorithms, we can now handle problems in which the coefficients vary by a factor of a thousand, from cell to cell, and can also handle exponentially stretched grids.

A variant of this code is being implemented on the Thinking Machines CM 2 at Los Alamos National Laboratory. While this class of multigrid algorithms is relatively communi-

cation intensive, it seems to map very nicely to SIMD parallel architectures. A hypercube version of this algorithm is also being considered, though the mapping issues involved are sufficiently different that plane relaxation algorithms may be superior on a hypercube.

David Nicol

We are studying "template" communication routing policies for SIMD parallelized numerical calculations with irregular communication patterns. We have identified conditions on the templates under which any work-conserving routing scheme is optimal, and have developed an algorithm which is optimal for a constrained class of templates.

In collaboration with A. Greenberg and B. Lubachevsky (AT&T Bell Labs), algorithms for executing trace-driven cache simulations on SIMD architectures are under study. We have developed algorithms suitable for simulating a general class of stack replacement policy algorithms, as well as random replacement. Previous results have been extended to include the efficient analysis of caches with very large set sizes.

In another effort, we are developing parallel MIMD and SIMD algorithms for the discrete-event simulation of networks where messages may be re-routed in the presence of network congestion.

Together with R. Simha (College of William and Mary) and D. Towsley (University of Massachusetts), we are looking at the application of the theory of majorization to problems in statically load balancing stochastically evolving workloads. Majorization permits us to assert that one mapping is better than another in a variety of ways, including expected execution time, variation in execution time, space-time product, and reliability.

Stephen Otto

The main concern of this study is a greater understanding of vortex wave interactions, particularly for situations involving the flow over a plate of variable curvature. We consider the imposition of a pressure gradient and the effect it has on the onset, and nonlinear development of a Görtler vortex mechanism. In joint work with P. Hall, we consider both incompressible and compressible boundary layers. We are interested primarily in finite amplitude vortices with small wavelengths, similar to those discussed in Hall & Lakin (1988). Also of considerable interest is the possibility that these flow situations may be susceptible to inviscid instabilities. For neutral Rayleigh waves to exist we require the flow field to include an inflection point. In the incompressible case this is only true if the pressure gradient takes a certain form. For a compressible flow situation we find that for high enough Mach numbers the flow may contain a generalised inflection point. It is possible to extend this analysis so

that the Rayleigh wave becomes large enough to alter the position of the vortex, although the wave itself remains linear in character. There is also interest in the verification of these results using fully numerical methods.

A weakly nonlinear study is being made on the effect of crossflow on the most dangerous Görtler mode, with a desire to extend this analysis to the fully nonlinear regime; this work is joint with A. P. Bassom (University of Exeter, UK).

Yuh-Roung Ou

In collaboration with J. Burns, the work concerning active control of unsteady flow by moving boundary mechanisms is continuing. An algorithm for computing the viscous flow past a rotating cylinder was developed for the purpose of studying the control of cylinder forces. Several fundamental types of rotation are demonstrated to be intimately relevant to the forces on the cylinder surface. Under a particular type of time-periodic rotation, a considerable improvement of the forces has been demonstrated. The computational results verify the significance of the proper choice of the rotation rate. Very precise periodicity of the force evolutions at certain cases are established, and it may provide direct implication for controlling the vortex formation in the cylinder wake. For the case of constant speed of rotation, two optimal control problems were considered and solved computationally.

By treating the rotation rate as a control variable in this model, we will eventually be interested in finding the optimal control (i.e. the optimal trajectory of the rotation rate) that maximizes the lift-to-drag ratio over a fixed time interval. Although in this study, an optimal control problem associated with the constant rotation rate was solved by direct computation, it is still important to explore further the implementation of a computational algorithm to calculate the optimal solution from the full necessary conditions. This approach may be applied to practical control problems arising in several areas of fluid flow.

Terry Pratt

A promising new method, called the KCD method, for automatic generation of an MIMD, distributed memory, parallel program from existing sequential code is being studied. The method is based on a theoretical model called "kernel-control decomposition" (KCD). The KCD method uses a source-to-source translation of the sequential code into a "control" process and multiple "kernel" processes. The control process determines the control path and assigns work (in the form of "kernel segments") to the kernel processes, which operate in parallel.

The KCD method has been applied to three applications codes to date, the NASA

LAURA code (Langley Aerothermodynamic Upwind Relaxation Algorithm), developed by P. Gnoffo (Space Systems Division, LaRC) and two of the codes distributed as part of the Perfect Club benchmark suite (FLO 52 and TRFD). Measurements of the performance of the parallel versions of these codes are being made on the 32-node NASA/ICASE Intel iPSC/860.

Peter Protzel

Together with D. Palumbo (Information Systems Division, LaRC) we have completed a study to investigate the potential benefits of using Artificial Neural Networks (ANNs) as components of critical, real time systems with high reliability requirements. The first part of this study considered an example of an application in which an ANN controlled the re-allocation of tasks in a fault-tolerant, distributed multiprocessor system. This reallocation is necessary if one of the processors fails and all tasks have to be distributed among the remaining processors as quickly as possible by observing certain constraints and by approximately balancing the load of the processors. Since the ANN becomes a critical component of the system in this application, we studied the fault-tolerance of the ANN by simulated fault-injection experiments. The results show a surprising degree of fault-tolerance with a graceful performance degradation even after multiple faults. Thus, an ANN implemented as an analog VLSI chip is an attractive alternative for performing certain critical functions, especially on long-term missions where cumulative component failures have to be expected without the possibility of repair or maintenance. More details on this application can be found in ICASE Report No. 91-45 and in a NASA Technical Paper currently in print.

The second part of our project focused on a different type of ANN to control the positioning of a robot arm with five degrees of freedom and with visual feedback provided by two cameras. This example application was chosen to demonstrate the fault-tolerance and adaptivity that can be achieved by using an ANN as the controller. The network learns and adapts on-line without any outside intervention. The continuous feedback provided by the cameras is used to generate an average positioning error that the networks tries to minimize. Three different issues were addressed from a fault-tolerant systems perspective; a possible (partial) failure of the controller, a failure of the robot arm, and a sudden change in the environmental or external conditions. In our simulations we showed, for example, how the system recovers from sudden failures of one or two arm joints, from a loss of 30% of the network's neurons, and from geometric changes in the camera positions. These remarkable results lead us to conclude that autonomous systems represent one of the most promising application areas for this kind of self-supervising ANN. Except for the fault-tolerance of the ANN itself, the main benefits can be achieved even if the ANN is only simulated and treated as an algorithm which can be executed by a standard microprocessor.

James Quirk

Work continued on the development of an adaptive grid algorithm for simulating shock hydrodynamic phenomena. Previously it was shown that the algorithm required only modest computing resources in order to produce very high resolution simulations. The basic efficiency of the algorithm stems from the fact that it refines in time as well as space. A larger number of smaller time steps are taken for fine mesh cells than for coarse mesh cells. Thus the scheme is inherently well suited to the task of producing time accurate simulations for flows which contain disparate length scales. However, a certain amount of geometric flexibility had been sacrificed so that the spatial and temporal refinement strategies could be linked harmoniously. Recent work has concentrated on removing this limitation.

Whereas in the past the algorithm essentially employed a body-fitted grid, it now uses a grid which intersects solid surfaces. In essence, a solid body is allowed to blank out areas of a cartesian grid. This results in a number of cut cells along the boundary of the solid which are meted out for special treatment during the integration of the flow solution. In principle such a strategy can cope with arbitrarily complicated bodies. Initial results are encouraging; at least for simple shapes such as wedges and cylinders the cut-cell approach produces results that are comparable to those produced by the body-fitted code. Further work is required to test this new approach on the sorts of complicated shapes that can be tackled routinely using unstructured grids.

Looking to the future, we intend to investigate the extent to which our adaptive grid algorithm can exploit the power offered by parallel computers, for this extent will have an important bearing on the long term usefulness of the scheme.

Rolf Radespiel and John Van Rosendale

Most flow solvers used in current aerospace programs exhibit slow convergence to the steady-state solution, resulting in high computer costs, large turn-around times, and slow progress towards the desired aerospace vehicle design. The reason is the appearance of flow phenomena with very different scales, also complicated by nonlinear behavior. Over the past several years, Radespiel has been developing a class of multigrid algorithms, using multiple semicoarsened grids, for the hypersonic regime. While the multiple coarse grids required are more expensive, such multigrid solvers appear much faster in the context of the Navier Stokes equations than traditional (full coarsening) multigrid solvers. The reason for this improvement seems to be that the multiple coarse grids effectively remove the stiffness arising from high aspect ratio cells in the boundary layer.

In order to understand such phenomena, we have been applying Fourier analysis to a two-level multigrid algorithm for the two-dimensional convection equation in collaboration

with C. Swanson (Fluid Mechanics Division, LaRC). This is yielding insight, though there are a number of complicating effects, including flow alignment issues, and the problem of the different speeds of convective and acoustic waves. The Runge Kutta "smoothers," used in Navier Stokes codes, are also difficult to analyze, since the smoother and the multigrid algorithm interact in complicated ways.

The two dimensional semicoarsening multigrid algorithms for the Navier Stokes equations developed so far are not directly usable in three dimensions, for several reasons. The primary reason is the great cost, in both storage and computation time, of all of the coarse grids required in three dimensions. In the elliptic case, a simple solution is to coarsen by a factor of four rather than two in each coordinate direction. Coarsening by a factor of two is expensive, since the multigrid algorithm requires eight times the amount of storage of the fine grid, and proportionately more work as well. Coarsening by a factor of four implies storage only about double that of the fine grid, but requires a better smoothing iteration, since more Fourier modes need to be effectively damped by the smoother.

In coming months we plan to implement a multigrid algorithm using the multiple coarse grids produced by factor of four coarsening in each coordinate direction, first for the elliptic case, then for the full Navier Stokes equations. In the elliptic case, we now have several effective ways of combining the corrections from the different coarse grids, all performing about equally well. This is not at all true in the hyperbolic case, where the way in which the results from the separate coarse grids are combined appears to be critical. The numerical test codes currently in progress should resolve the issue of how best to do this.

Dan Reed and David Nicol

We are developing simulation models and analytic models of dynamic load-balancing policies that choose a destination processor at random. Such policies are easy to implement, although they ignore state information. Our aim is to assess the quality and costs of these types of policies.

Philip Roe

I concentrated on clarifying the scalar update algorithms for use in the new class of multidimensional upwind schemes. This led to a unification of previous work and to some estimates of truncation error for both the linear and nonlinear cases.

I also did some preliminary work to explore the use of CFD methods for aeroacoustic problems, and looked at a promising technique for solving the steady Navier-Stokes equations by fast explicit methods.

Joel Saltz, Scott Berryman, Raja Das, Dimitri Mavriplis, Vijay Naik, Ravi Ponnusamy and Sesh Venugopal

We have further developed and refined Fortran and C callable distributed memory PARTI procedures to carry out execution time preprocessing needed for sparse matrix and unstructured mesh problems. Our new optimizations include methods for increasing the number of situations in which it is simple to avoid communication by reusing stored off-processor data. We also have developed a suite of primitives that track runtime data dependencies. These primitives are useful in such problems as sparse direct methods. We have used our new primitives to implement on the iPSC/860 applications such as Mavriplis' 3-D unstructured mesh explicit and multigrid Euler solver, Horst Simon's recursive spectral domain partitioner, a conjugate gradient solver, a substantial portion of the molecular dynamics program CHARMM and a sparse direct systems solver.

The explicit Euler solver on a 210K mesh carries out calculations at a rate in excess of 160 Mflops on 64 processors. The multigrid Euler solver carries out calculations at a rate in excess of 130 Mflops on 64 processors. Most of the time in both calculations is spent on computation. We have promising results that indicate that reordering the data and loop iterations will lead to a significant improvement in computational rates. The explicit unstructured Euler solver has been ported to the Delta machine at CalTech; performance studies are under way.

The primitives are available now from netlib or by anonymous ftp from ra.cs.yale.edu. A manual for some primitives is available as ICASE Interim report 91-17, other manuals are pending.

Joel Saltz, Craig Chase and Kay Crowley

Fortran and C callable procedures which carry out symbolic and execution time preprocessing needed for data exchange in block structured and structured adaptive programs are under study. We have developed a new suite of primitives for block structured and structured adaptive problems and have tested the primitives using routines from the block structured Navier Stokes code written by V. Vatsa (Fluid Mechanics Division, LaRC). We have also developed a rudimentary compiler capable of generating code that runs on distributed memory processors. This compiler has been tested for simple block structured kernels.

Earlier versions of the primitives were used in a structured adaptive PDE solver developed by J. Scroggs; currently the primitives are being used to implement a NASA block structured Euler solver. The primitives are being used to implement and extend Fortran D in joint work with the groups of Ken Kennedy and Geoffrey Fox at the NSF Center for Research on Parallel Computing.

Joel Saltz, Raja Das and Ravi Ponnusamy

We have developed two methods which we believe will play an important role in any distributed memory compiler able to handle sparse and unstructured problems. We described in ICASE report 91-73 how to link runtime partitioners to distributed memory compilers. In our scheme, programmers can *implicitly* specify how data and loop iterations are to be distributed between processors. This insulates users from having to deal explicitly with potentially complex algorithms that carry out work and data partitioning.

In ICASE report 91-73 we also described a viable mechanism for tracking and reusing copies of off-processor data. In many programs, several loops access the same off-processor memory locations. As long as it can be verified that the values assigned to off-processor memory locations remain unmodified, we showed that we can effectively reuse stored off-processor data. We presented experimental data from a 3-D unstructured Euler solver run on an iPSC/860 to demonstrate the usefulness of our methods.

The Parti primitives can be used directly by programmers or incorporated into compiler for distributed memory architectures. They are currently being used to implement and extend Fortran D in joint work with K. Kennedy, C. Koelbel and R. von Hanxleden (Rice University) and G. Fox and A. Choudhary (Syracuse University).

Joel Saltz and Satyanarayan Gupta

We have developed PARTI primitives for the Maspar and have used these primitives to implement Dimitri Mavriplis' 3-D explicit unstructured Euler code. The Parti code must preprocess message patterns in a manner that allows the Maspar router to be effectively used. We are currently investigating heuristics that can be used to carry out this preprocessing.

Sutanu Sarkar

We are engaged in the direct simulation and Reynolds stress modeling of turbulent flows. Our simulations of homogeneous shear flow show that compressibility leads to a significant decrease in the growth rate of turbulent kinetic energy. Augmented dissipation (through the dilatational dissipation) and energy transfer to pressure fluctuations (through the pressure-dilatation) have been identified as mechanisms responsible for the decreased growth rate. Furthermore, we have proposed an algebraic model for the pressure-dilatation to be used in Reynolds stress modeling of high-speed flows. To complement the non-linear direct simulations, we have also studied the linear stability of compressible homogeneous shear flow.

Compressibility effects on turbulence structure are now being obtained in collaboration with G. Erlebacher by analysis of the shear flow simulations. We are also addressing issues related to turbulence anisotropy and pressure-strain modeling for compressible shear flows.

Jeffrey S. Scroggs and Peter A. Jacobs

An algorithm is being developed for the driver of a multi-domain PDE solver, with target application being the time-accurate simulation of high-speed gasdynamics using structured grids for each of the domains. The driver algorithm uses a time-accurate solver for a single block essentially as a black-box. In addition to the physical boundary conditions, multidomain solvers require sharing information at the (artificial) interfaces between domains. We allow different time steps to be taken on adjacent grids. When $\Delta t_i/\Delta t_j > 1$, we interpolate the solution from grid j to grid i , and will use a flux-correction scheme to share data from grid i to grid j . The interpolation has been implemented, and the implementation of the flux-correction is a subject of current research.

We demonstrated multi-driver for a three-block decomposition of axi-symmetric flow around the leading edge of a cone using the single-block integrator described in previous reports by P. Jacobs.

Sharon O. Seddougui

The instability of hypersonic flow past a cone is being investigated with A. Bassom (University of Exeter). The effect of an attached shock is studied in the weak interaction region. We find that the triple deck structure is identical to that given by Cowley and Hall (1990) for hypersonic flow over a wedge. In this case the local position on the cone is determined so that the effects of curvature are important. Solutions of the dispersion relation are currently being obtained. Joint work with A. Bassom was completed investigating the effect of suction on the stability of the viscous stationary modes for the flow over a rotating disc. MacKerrell (1988) showed that this crossflow instability is subcritical, and that there exists a threshold value of the disturbance amplitude. We show that suction does not alter these results although it lowers the value of the threshold amplitude. Thus suction increases the likelihood of this mode in an experimental setting. Asymptotic results for large suction and large blowing were obtained. The extension of this problem into the compressible regime is currently being studied.

Charles G. Speziale

An analysis of the Renormalization Group (RNG) $K - \epsilon$ model of Yakhot & Orszag was conducted in collaboration with T.B. Gatski (Fluid Mechanics Division, LaRC) and S. Thangam. It was found that with a correction of the numerical value of one of the constants – and with the incorporation of a nonlinear strain dependent modification to the production of dissipation term – a substantially better description of turbulent shear flows was achieved. In particular, excellent predictions were obtained for homogeneous shear flow and turbulent flow over a backward facing step: two test cases that are commonly used to benchmark the performance of turbulence models. Future research is planned on the development of further modifications that will allow this two-equation model to fully accommodate the rapid distortion limit.

Research was conducted in collaboration with P.S. Bernard (University of Maryland) on the theory of self-preservation in homogeneous turbulence. It was found that self-preservation renders an alternative equilibrium structure which includes a t^{-1} asymptotic power law decay in isotropic turbulence and a production-equals-dissipation equilibrium in homogeneous shear flow. The ability of the self preserving model to accommodate the limit of zero viscosity – wherein it predicts a finite time enstrophy blow up – allows for a better description of non-equilibrium turbulent flows. Applications of these results to the development of improved turbulence models are currently under investigation.

A new near-wall two-equation turbulence model for supersonic flows has been developed in collaboration with R.M.C. So (Arizona State University). A variable density extension of the asymptotically consistent near-wall model of So and co-workers for incompressible flows is combined with some new dilatational models developed recently by S. Sarkar. Excellent results are obtained in the supersonic flat plate turbulent boundary layer for Mach numbers as large as 10. Future research is planned where this approach will be extended to second-order closure models.

Shlomo Ta'asan

The development of efficient multigrid solvers for constraint optimization problems governed by partial differential equations has continued with research in two directions. The first, which is well developed by now, deals with problems in which the parameter space on which optimization is done is of finite dimension in the differential formulation of the problem. The methods use relaxation for the parameter space in a multilevel way. Parameters that have a non-smooth effect on the solution are relaxed on fine levels while those of smooth effect are solved for on coarse grids only. The methods use adjoint variables to define a descent direction for the minimization problem. The other direction focuses on

problems in which the optimization is over an infinite dimensional parameter space (in the differential level). Also here the same type of ideas for the treatment of the different scales in the problems is being used. Experiments with some model problems involving elliptic partial differential equations as the constraint equations have been performed showing that the full optimization problem can be solved with a computational cost which is only a few times more than that of solving the PDE alone.

The above ideas have been applied in aerodynamics design problems where airfoils are to be calculated so as to meet certain design requirements, for example, to give pressure distribution in some flow conditions which are closest to a given pressure distribution. The present model for the flow is the transonic small disturbance equation in which an airfoil is modelled by the small disturbance boundary condition. The shape of the airfoil in these calculations is being expressed in terms of a finite number of given shape functions with amplitudes to be found by the design process. We have shown that subsonic design problems can be solved in a computational cost which is just a few times (2-3) that of the flow solver. This work is jointly done with M. D. Salas (Fluid Dynamics Division, LaRC) and G. Kuruvila (Vigyan, Inc.).

New multigrid solvers for inviscid flow problems are being developed in which the convergence rates are to be like that of the full potential equation. These convergence rates have been predicted by Fourier analysis. These solvers employ relaxation methods of the Gauss-Seidel type with a proper modification to handle systems of partial differential equations. At present we focus on the incompressible inviscid case, working with body fitted grids in two dimension, using MAC discretization schemes.

Another area of research is the development of new computational techniques in elastic-plastic problems. Here a set of non-linear equations which involve also weak dependence of the history of the loading are to be calculated. A new numerical scheme for the integration of the plastic forces has been constructed. Using this scheme an efficient multigrid solver is under investigation. It uses appropriate fine to coarse grid transfer of the yield functions so as to enable the solution of the large scale behavior of the plastic forces to be done on the coarsest levels, yielding the accuracy of the fine grid solution. The method is under study with some real elastic-plastic problems related to the understanding of fatigue failure in metals. The convergence rates that are obtained with the present formulation of the algorithm are not satisfactory, i.e., much slower than the linear case. Further investigation will focus on understanding this point.

Siva Thangam

Turbulent separated flow past a backward-facing step is considered from modeling, com-

putational and experimental point of view. The first and the second phases of this collaborative effort involving C. Speziale, M.Y. Hussaini and S. Kjelgaard (Fluid Mechanics Division, LaRC) have been completed. In the first phase, the equations of motion based on the two-equation Reynolds stress closure model are solved using a finite-volume algorithm. The results show that when the boundary conditions are consistently applied, the experimental and computational results are in very good agreement. During the second phase, several refinements were made to the two-equation ($k-\epsilon$) model to improve its predictive capability. It was ascertained that the optimal selection of the model constants, inclusion of anisotropy, or the accurate representation of the turbulence production-dissipation balance, can considerably improve the two-equation model predictions. Computations were also performed using the large-eddy simulation method with an eddy-viscosity based subgrid scale model. The predictions of the time-averaged results of the large-eddy simulation (with $96 \times 48 \times 32$ mesh) were compared with the available experimental findings as well as with those from the two-equation model computations (based on a 100×50 mesh) for a step to channel height ratio of 1:3. It was found that the dominant features of the flow field – namely, the size of the separated flow region and the mean velocity profiles – can be accurately predicted. In addition, during this phase the construction and testing of the backward-facing step facility at the Experimental Methods Branch was completed. During the next phase, detailed experiments as well as additional computations based on full Reynolds-stress closure model and large-eddy simulations will be performed for a variety of flow conditions. The issues involving the the subgrid scale representation for the large-eddy simulations as well as the predictive capability of the full-Reynolds stress closure model will be addressed.

Eli Turkel

Work was continued on extensions of central difference and multigrid techniques to hypersonic problems. The standard method does not converge due to the presence of strong shocks. By revising the switch near shocks and using residual smoothing on the way to finer meshes, converged solutions with good convergence rates were obtained for Mach 10 and Mach 20 turbulent flows about many aerodynamic bodies including the HSCT project. A sequence of ICASE reports were written for various applications.

A new project was begun in constructing new implicit schemes for spectral methods that are easier to invert than a full implicit trapezoidal rule or backward Euler. These methods are only first order accurate for time dependent problems but spectrally accurate for steady state problems. In some simple test cases on the one dimensional Euler equations the algorithm

converged to the steady state within four time steps on a mesh with 64 nodes using the pseudospectral Chebyshev method. The algorithm is currently being extended to two space dimensions.

Bram van Leer

The work on a multi-dimensional approximate Riemann solver with C. Rumsey (Fluid Mechanics Division, LaRC) was completed with Rumsey's doctoral thesis at the University of Michigan. Although some very good results and insights have been obtained, it is felt that in this work the amount of information extracted from the two input states is too large to lead to a robust method. In particular, the use of the input data to define a rotated coordinate frame in which the Riemann problem based on the same input data is then solved, leads to noisy, unsteady solutions where a steady solution should be found. Although one still can think of some modifications that are worth trying, these will presently not be implemented.

The work on local preconditioning of the Euler equations continued in collaboration with E. Turkel, and led to quite a surprise: one matrix of a family derived earlier by Turkel has exactly the same effect on the wave speeds as the preconditioning matrix derived by Van Leer, Lee and Roe. The matrices are different: Van Leer's is symmetric for the symmetrized Euler equations, while Turkel's is not. There probably is a whole two-parameter family of matrices that can achieve the optimal characteristic condition number; an explicit formula for these has not yet been obtained. Further work on the preconditioning matrix for stretched grids is underway. It is possible to overcome, at least in part, the stiffness caused by the presence of strongly elongated cells, such as found in boundary layers. While the use of the preconditioning for the Navier-Stokes equations still has to be explored, the matter of the large cell aspect-ratio can be studied independently with Euler schemes used on Navier-Stokes type grids.

Sesh Venugopal

One of the objectives of the work with J. Saltz and V. Naik, (I.B.M. T.J. Watson Research Center.) in progress is to develop a new set of efficient primitives for automating the communication during the execution of a task dependency directed acyclic graph (DAG). These primitives are designed for run-time support of any computation whose communication can be expressed as a coarse-grained DAG, with the nodes in the DAG representing linear blocks of data. As a test DAG, we have considered the column oriented sparse Cholesky factorization algorithm. I have implemented four versions of this algorithm on the iPSC/860 and have obtained execution timings for each. One of the versions is based on dynamic

task scheduling while the other three use a static or pre-determined ordering of tasks on processors. One of the static versions uses PARTI primitives for message passing, another performs manual communication and the third uses the new DAG primitives.

A second objective of this work is to determine the effects of partitioning and scheduling of sparse factorization on load balancing and communication (ICASE Report No. 91-80). Work is continuing towards developing efficient block partitioning and scheduling schemes. We plan to implement the block factorization code on the iPSC/860 and compare its performance with column based codes, and extend the DAG primitives to handle higher dimensional blocks of data.

Hans Zima, Piyush Mehrotra and Barbara Chapman

In recent years, a number of distributed memory multiprocessing computers have been introduced into the market (e.g. Intel's iPSC series, NCUBE, and several transputer based systems). In contrast to shared memory machines, these architectures are less expensive to build and are potentially scalable to a large number of processors. However, the associated programming paradigm requires the user to specify complete details of the synchronization and the communication of data between processors as dictated by the algorithm. Experience has shown that forcing the user to provide such low level details not only makes distributed memory programming tedious and error prone but also inhibits experimentation.

Based on our earlier work on languages and compilers for distributed memory machines, we have been investigating machine-independent language extensions for FORTRAN 77, called Vienna Fortran (ICASE Report 91-2). These extensions allow the user to write programs for distributed memory architectures using global data references only. Since the distribution of data to the processors is critical for performance, the extensions described here permit the user to explicitly control the mapping of data onto the processors. Vienna Fortran supports a wide range of facilities for specifying data distributions, including distribution by alignment, where one array is mapped so that it has a fixed relationship with another array. It also supports dynamic redistribution of data. Frequently occurring distributions can be specified in a simple manner, whereas the full language permits complex mappings. The overall aim of the language extensions provided by Vienna Fortran is to make the transition from the sequential algorithm to a parallel version as easy as possible, without sacrificing performance.

REPORTS AND ABSTRACTS

Banks, H.T., G. Propst, and R.J. Silcox: *A comparison of time domain boundary conditions for acoustic waves in wave guides*. ICASE Report No. 91-27, August 15, 1991, 25 pages. Submitted to Journal of Sounds and Vibration.

We consider several types of boundary conditions in the context of time domain models for acoustic waves. Experiments with four different duct terminations (hardwall, free radiation, foam, wedge) were carried out in a wave duct from which reflection coefficients over a wide frequency range were measured. These reflection coefficients are used to estimate parameters in the time domain boundary conditions and a comparison of the relative merits of the models in describing the data is presented. Boundary conditions which yield a good fit of the model to the experimental data were found for all duct terminations except the wedge.

Lasseigne, D. G., T. L. Jackson, and M. Y. Hussaini: *Non-linear interaction of a detonation/vorticity wave*. ICASE Report No. 91-34, April 1, 1991, 27 pages. To appear in Physics of Fluids A.

The interaction of an oblique, overdriven detonation wave with a vorticity disturbance is investigated by a direct two-dimensional numerical simulation using a multi-domain, finite-difference solution of the compressible Euler equations. The results are compared to those of linear theory, which predict that the effect of exothermicity on the interaction is relatively small except possibly near a critical angle where linear theory no longer holds. It is found that the steady-state computational results whenever obtained in this study agree with the results of linear theory. However, for cases with incident angle near the critical angle, moderate disturbance amplitudes, and/or sudden transient encounter with a disturbance, the effects of exothermicity is more pronounced than predicted by linear theory. Finally, it is found that linear theory correctly determines the critical angle.

Grosch, C. E., and T. L. Jackson: *Ignition and structure of a laminar diffusion flame in a compressible mixing layer with finite rate chemistry*. ICASE Report No. 91-35, April 8, 1991, 28 pages. Submitted to Physics of Fluids A.

In this paper we consider the ignition and structure of a reacting compressible mixing layer using finite rate chemistry lying between two streams of reactants with different freestream speeds and temperatures. Numerical integration of the governing equations show that the structure of the reacting flow can be quite complicated depending on the magnitude of the Zeldovich number. In particular, for sufficiently large Zeldovich number, the three regimes first described by Linan and Crespo (1976); ie., ignition, deflagration, and diffusion flame, occur in supersonic as well as in subsonic flows. An analysis of both the ignition and diffusion flame regimes is presented using a combination of large Zeldovich number asymptotics and numerics. This allows us to analyze the behavior of these regimes as a function of the parameters of the problem. For the ignition regime, a well defined ignition point will always exist provided the adiabatic flame temperature is greater than either freestream temperature.

One important result is that at supersonic speeds ignition occurs far downstream from the plate and, as the flow is accelerated to hypersonic speeds, ignition is exponentially delayed. For the diffusion flame regime, the location of the flame changes significantly with changes in the equivalence ratio and the Schmidt numbers.

Thompson, C. P., G. K. Leaf, and J. Van Rosendale: *A dynamically adaptive multigrid algorithm for the incompressible Navier-Stokes equations - Validation and model problems*. ICASE Report No. 91-36, June 27, 1991, 32 pages. Submitted to J. of Applied Numerical Mathematics.

We describe an algorithm for the solution of the laminar, incompressible Navier-Stokes equations. The basic algorithm is a multigrid method based on a robust, box-based smoothing step. Its most important feature is the incorporation of automatic, dynamic mesh refinement. Using an approximation to the local truncation error to control the refinement, we use a form of domain decomposition to introduce patches of finer grid wherever they are needed to ensure an accurate solution. This refinement strategy is completely local: regions that satisfy our tolerance are unmodified, except when they must be refined to maintain reasonable mesh ratios. This locality has the important consequence that boundary layers and other regions of sharp transition do not (lqsteal(rq mesh points from surrounding regions of smooth flow, in contrast to moving mesh strategies where such (lqstealing(rq is inevitable.

Our algorithm supports generalized simple domains, that is, any domain defined by horizontal and vertical lines. This generality is a natural consequence of our domain decomposition approach. We base our program on a standard staggered-grid formulation of the Navier-Stokes equations for robustness and efficiency. To ensure discrete mass conservation, we have introduced special grid transfer operators at grid interfaces in the multigrid algorithm. While these operators complicate the algorithm somewhat, our approach results in exact mass conservation and rapid convergence.

In this paper, we present results for three model problems: the driven-cavity, a backward-facing step, and a sudden expansion/contraction. Our approach obtains convergence rates that are independent of grid size and that compare favorably with other multigrid algorithms. We also compare the accuracy of our results with other benchmark results.

Speziale, Charles G., Thomas B. Gatski, and Nessim Fitzmaurice: *An analysis of RNG based turbulence models for homogeneous shear flow*. ICASE Report No. 91-37, April 16, 1991, 12 pages. To be submitted to Physics of Fluids A.

In a recent paper [*Phys. Fluids* A2:1678-1684, 1990], the authors compared the performance of a variety of turbulence models including the $K - \epsilon$ model and the second-order closure model derived by Yakhot and Orszag based on Renormalization Group (RNG) methods. The performance of these RNG models in homogeneous turbulent shear flow was found to be quite poor, apparently due to the value of the constant $C_{\epsilon 1}$ in the modeled dissipation rate equation which was substantially lower than its traditional value. However, recently a correction has been made in the RNG based calculation of $C_{\epsilon 1}$. It is shown herein that with the new value of $C_{\epsilon 1}$, the performance of the RNG $K - \epsilon$ model is substantially improved. On the other hand, while the predictions of the revised RNG second-order closure model are better, some lingering problems still remain which can be easily remedied by the addition of higher-order terms.

Shu, Chi-Wang, Gordon Erlebacher, Thomas A. Zang, David Whittaker, and Stanley Osher: *High-order ENO schemes applied to two- and three-dimensional compressible flow*. ICASE Report No. 91-38, April 30, 1991, 44 pages. Submitted to J. Applied Numerical Mathematics.

High-order essentially non-oscillatory (ENO) finite-difference schemes are applied to the two- and three-dimensional compressible Euler and Navier-Stokes equations. Practical issues, such as vectorization, efficiency of coding, cost comparison with other numerical methods and accuracy degeneracy effects, are discussed. Numerical examples are provided which are representative of computational problems of current interest in transition and turbulence physics. These require both non-oscillatory shock capturing and high resolution for detailed structures in the smooth regions and demonstrate the advantage of ENO schemes.

Fu, Yibin B., and Philip Hall: *Nonlinear development and secondary instability of Görtler vortices in hypersonic flows*. ICASE Report No. 91-39, May 2, 1991, 47 pages. Submitted to Euro. J. of Mechanics.

In a hypersonic boundary layer over a wall of variable curvature, the region most susceptible to Görtler vortices is the temperature adjustment layer over which the basic state temperature decreases monotonically to its free stream value (Hall & Fu (1989), Fu, Hall & Blackaby (1990)). Except for a special wall curvature distribution, the evolution of Görtler vortices trapped in the temperature adjustment layer will in general be strongly affected by boundary layer growth through the $O(M^{3/2})$ curvature of the basic state, where M is the free stream Mach number. Only when the local wavenumber becomes as large as of order $M^{3/8}$, do nonparallel effects become negligible in the determination of stability properties. In the latter case, Görtler vortices will be trapped in a thin layer of $O(\epsilon^{1/2})$ thickness which is embedded in the temperature adjustment layer; here ϵ is the inverse of the local wavenumber. In this paper, we first present a weakly nonlinear theory in which the initial nonlinear development of Görtler vortices in the neighbourhood of the neutral position is investigated and two coupled evolution equations are derived. From these two evolution equations we can determine whether the vortices are decaying or growing depending on the sign of a constant which is related to the wall curvature and the basic state temperature. In the latter case, it is found that the mean flow correction becomes as large as the basic state at distances $O(1)$ downstream of the neutral position. Next, we present a fully nonlinear theory concerning the further downstream development of these large-amplitude Görtler vortices. It is shown that the vortices spread out across the boundary layer. The upper and lower boundaries of the region of vortex activity are determined by a free-boundary problem involving the boundary layer equations. Finally, the secondary instability of the flow in the transition layers located at the upper and lower edges of the region of vortex activity is considered. The superimposed wavy vortex perturbations are spanwise periodic travelling waves which are $\pi/2$ radians out of phase with the fundamental. The dispersion relation is found to be determined by solving two coupled differential equations and it is shown that an infinite number of neutrally stable modes may exist.

Venkatakrishnan, V., and Dimitri J. Mavriplis: *Implicit solvers for unstructured meshes*. ICASE Report No. 91-40, May 6, 1991, 23 pages.

We develop and test implicit methods for unstructured mesh computations. The approximate system which arises from the Newton-linearization evolution operator is solved by using the preconditioned GMRES (Generalized Minimum Residual) technique. We investigate three different preconditioners, namely, the incomplete LU factorization (ILU), block diagonal factorization and the symmetric successive over-relaxation (SSOR). The preconditioners have been optimized to have good vectorization properties. We also study SSOR and ILU themselves as iterative schemes. The various methods are compared over a wide range of problems. Ordering of the unknowns, which affects the convergence of these sparse matrix iterative methods, is also investigated. Results are presented for inviscid and turbulent viscous calculations on single and multi-element airfoil configurations using globally and adaptively generated meshes.

Mavriplis, D. J.: *Three dimensional unstructured multigrid for the Euler equations*. ICASE Report No. 91-41, May 7, 1991, 29 pages. Submitted to AIAA Journal.

The three-dimensional Euler equations are solved on unstructured tetrahedral meshes using a multigrid strategy. The driving algorithm consists of an explicit vertex-based finite-element scheme, which employs an edge-based data-structure to assemble the residuals. The multigrid approach employs a sequence of independently generated coarse and fine meshes to accelerate the convergence to steady-state of the fine grid solution. Variables, residuals and corrections are passed back and forth between the various grids of the sequence using linear interpolation. The addresses and weights for interpolation are determined in a preprocessing stage using an efficient graph traversal algorithm. The preprocessing operation is shown to require a negligible fraction of the CPU time required by the overall solution procedure, while gains in overall solution efficiencies greater than an order of magnitude are demonstrated on meshes containing up to 350,000 vertices. Solutions using globally regenerated fine meshes as well as adaptively refined meshes are given.

Sarkar, S.: *Modeling the pressure-dilatation correlation*. ICASE Report No. 91-42, May 7, 1991, 20 pages. Submitted to Physics of Fluids A.

It is generally accepted that the pressure-dilatation, which is an additional compressibility term in the turbulence transport equations, may be important for high-speed flows. Recent direct simulations of homogeneous shear turbulence have given concrete evidence that the pressure-dilatation is important insofar that it contributes to the reduced growth of turbulent kinetic energy due to compressibility effects. The present work addresses the problem of modeling the pressure-dilatation. We first isolate a component of the pressure-dilatation which exhibits temporal oscillations and, using direct numerical simulations of homogeneous shear turbulence and isotropic turbulence, show that it has a negligible contribution to the evolution of turbulent kinetic energy. Then, an analysis for the case of homogeneous turbulence is performed to obtain a model for the non-oscillatory pressure-dilatation. This model algebraically relates the pressure-dilatation to quantities traditionally obtained in incompressible turbulence closures. The model is validated by direct comparison with the pressure-dilatation data obtained from the simulations.

Smith, Ralph C., and Kenneth L. Bowers: *Sinc-Galerkin estimation of diffusivity in parabolic problems*. ICASE Report No. 91-43, May 7, 1991, 36 pages. Submitted to Inverse Problems.

A fully Sinc-Galerkin method for the numerical recovery of spatially varying diffusion coefficients in linear parabolic partial differential equations is presented. Because the parameter recovery problems are inherently ill-posed, an output error criterion in conjunction with Tikhonov regularization is used to formulate them as infinite-dimensional minimization problems. The forward problems are discretized with a sinc basis in both the spatial and temporal domains thus yielding an approximate solution which displays an exponential convergence rate and is valid on the infinite time interval. The minimization problems are then solved via a quasi-Newton/trust region algorithm. The L -curve technique for determining an appropriate value of the regularization parameter is briefly discussed, and numerical examples are given which demonstrate the applicability of the method both for problems with noise-free data as well as for those whose data contains white noise.

Hall, Philip, and Helen Morris: *On the instability of boundary layers on heated flat plates*. ICASE Report No. 91-44, May 29, 1991, 71 pages. To be submitted to Journal of Fluid Mechanics.

The stability of a boundary layer on a heated flat plate is investigated in the linear regime. The flow is shown to be unstable to longitudinal vortex structures which in general develop in a nonparallel manner in the streamwise direction. Solutions of the nonparallel equations are obtained numerically at $O(1)$ values of the appropriate stability parameter, ie the Grashof number. The particular cases investigated relate to the situations when the instability is induced by localized or distributed wall roughness or nonuniform wall heating. The case when the vortices are induced by freestream disturbances is also considered. The fastest growing mode is found to be governed by a quasi-parallel theory at high wavenumbers. The wavenumber and growth rate of the fastest growing mode are found in closed form. At low wavenumbers the vortex instability is shown to be closely related to Tollmein-Schlichting waves, the effect of wall heating or cooling on the latter type of instability is discussed.

Protzel, Peter W., Daniel L. Palumbo, and Michael K. Arras: *Performance and fault-tolerance of neural networks for optimization*. ICASE Report No. 91-45, June 6, 1991, 33 pages. Submitted to IEEE Transactions on Neural Networks.

One of the key benefits of future hardware implementations of certain Artificial Neural Networks (ANNs) is their apparently "built-in" fault-tolerance, which makes them potential candidates for critical tasks with high reliability requirements. This paper investigates the fault-tolerance characteristics of time-continuous, recurrent ANNs that can be used to solve optimization problems. The performance of these networks is first illustrated by using well-known model problems like the Traveling Salesman Problem and the Assignment Problem. The ANNs are then subjected to up to 13 simultaneous "stuck-at-1" or "stuck-at-0" faults for network sizes of up to 900 "neurons." The effect of these faults on the performance is demonstrated and the cause for the observed fault-tolerance is discussed. An application is presented in which a network performs a critical task for a real-time distributed processing system by generating new task allocations during the reconfiguration of the system. The

performance degradation of the ANN under the presence of faults is investigated by large-scale simulations and the potential benefits of delegating a critical task to a fault-tolerant network are discussed.

Bryan, Kurt, and Michael Vogelius: *A uniqueness result concerning the identification of a collection of cracks from finitely many electrostatic boundary measurements*. ICASE Report No. 91-46, June 11, 1991, 18 pages. Submitted to SIAM Journal of Mathematical Analysis.

We consider the problem of locating and identifying a collection of finitely many cracks inside a planar domain from measurements of the electrostatic boundary potentials induced by specified current fluxes. It is shown that a collection of n or fewer cracks can be uniquely identified by measuring the boundary potentials induced by $n + 1$ specified current fluxes, consisting entirely of electrode pairs.

Banks, H.T., K. Ito, and C. Wang: *Exponentially stable approximations of weakly damped wave equations*. ICASE Report No. 91-47, June 11, 1991, 40 pages. To appear in Proceedings of the International Conference on Control of DPS, Voran (July 1990), Birkhäuser.

We consider wave equations with damping in the boundary conditions. Techniques to ascertain the uniform preservation under approximation of exponential stability are presented. Several schemes for which preservation can be guaranteed are analyzed. Numerical results that demonstrate the lack of stability under approximation for several popular schemes (including standard finite difference and finite element schemes) are given.

Banks, H.T., D. Cioranescu, A. Das, R. Miller and D.A. Rebnord: *Homogenization techniques and estimation of material parameters in distributed structures*. ICASE Report No. 91-48, June 12, 1991, 24 pages. To appear in Proc. 2nd Conf. on Computational Control, Birkhäuser, (August 1991).

We discuss the use of homogenization techniques to derive approximate models with simple geometry for physical models of grids and trusses which have a complex geometry that gives rise to computational difficulties. Our presentation is in the context of inverse or parameter estimation problems for composite material structures with unknown characteristics such as stiffness and internal damping. We present the necessary theoretical foundations for this approach and discuss comparison of modal properties of the resulting homogenization model for a two-dimensional grid structure with modal properties observed in experiments with this grid.

Ou, Yuh-Roung, and John A. Burns: *Optimal control of lift/drag ratios on a rotating cylinder*. ICASE Report No. 91-49, June 14, 1991, 13 pages. Submitted to Applied Mathematics Letters.

We present the numerical solution to a problem of maximizing the lift to drag ratio by rotating a circular cylinder in a two-dimensional viscous incompressible flow. This problem is viewed as a test case for the newly developing theoretical and computational methods for control of fluid dynamics systems. We show that the time averaged lift to drag ratio for a fixed finite-time interval achieves its maximum value at an optimal rotation rate that depends on the time interval.

Duck, Peter W.: *The unsteady laminar boundary layer on an axisymmetric body subject to small amplitude fluctuations in the free-stream velocity*. ICASE Report No. 91-50, June 20, 1991, 43 pages. To appear in J. Fluid Mechanics.

The effect of small amplitude, time-periodic, freestream disturbances on an otherwise steady axisymmetric boundary layer on a circular cylinder is considered. Numerical solutions of the problem are presented, and an asymptotic solution, valid far downstream along the axis of the cylinder is detailed. Particular emphasis is placed on the unsteady eigensolutions that occur far downstream, which turn out to be very different from the analogous planar eigensolutions. These axisymmetric eigensolutions are computed numerically and also are described by asymptotic analyses valid for low and high frequencies of oscillation.

Lasseigne, D. G., and T. L. Jackson: *Stability of a non-orthogonal stagnation flow to three dimensional disturbances*. ICASE Report No. 91-51, June 20, 1991, 28 pages. To appear in Theoretical and Computational Fluid Dynamics.

A similarity solution for a low Mach number non-orthogonal flow impinging on a hot or cold plate is presented. For the constant density case, it is known that the stagnation point shifts in the direction of the incoming flow and that this shift increases as the angle of attack decreases. When the effects of density variations are included, a critical plate temperature exists; above this temperature the stagnation point shifts away from the incoming stream as the angle is decreased. This flow field is believed to have applications to the reattachment zone of certain separated flows or to a lifting body at a high angle of attack. Finally, we examine the stability of this non-orthogonal flow to self-similar, three dimensional disturbances. Stability characteristics of the flow are given as a function of the parameters of this study: ratio of the plate temperature to that of the outer potential flow and angle of attack. In particular, it is shown that the angle of attack can be scaled out by a suitable definition of an equivalent wavenumber and temporal growth rate, and the stability problem for the non-orthogonal case is identical to the stability problem for the orthogonal case. By use of this scaling, it can be shown that decreasing the angle of attack decreases the wavenumber and the magnitude of the temporal decay rate, thus making nonlinear effects important. For small wavenumbers it is shown that cooling the plate decreases the temporal decay of the least stable mode, while heating the plate has the opposite effect. For moderate to large wavenumbers, density variations have little effect except that there exists a range of cool plate temperatures for which these disturbances are extremely stable.

Overman, Andrea L., and John Van Rosendale: *Mapping implicit spectral methods to distributed memory architectures*. ICASE Report No. 91-52, June 28, 1991, 9 pages. To appear in Proc. 5th SIAM Conf. on Parallel Computing, Houston, TX, March 1991.

Spectral methods have proven invaluable in numerical simulation of PDEs, but the frequent global communication required raises a fundamental barrier to their use on highly parallel architectures. To explore this issue, we implemented a three dimensional implicit spectral method on an Intel hypercube. Utilization of about 50% was achieved on a 32 node iPSC/860 hypercube, for a $64 \times 64 \times 64$ Fourier-spectral grid; finer grids yield higher utilizations.

Chebyshev-spectral grids are more problematic, since plane-relaxation based multigrid is required. However, by using a semicoarsening multigrid algorithm, and by relaxing all multigrid levels concurrently, relatively high utilizations were also achieved in this harder case. In fact, since the amount of work per processor was higher in this case, we achieved somewhat higher utilization, typically 60% on moderate sized problems. Thus spectral methods remain attractive on the current generation of distributed memory architectures.

Tanveer, S.: *Evolution of a Hele Shaw interface for small surface tension*. ICASE Report No. 91-53, June 28, 1991, 63 pages. Submitted to Phil. Trans. Roy. Soc. London.

We present analytical evidence suggesting that for zero surface tension, the initial value problem for a Hele-Shaw flow described by a conformal map $z(\zeta, t)$ at time t from inside the unit ζ semi-circle (or unit circle for a radial geometry) to the physical flow domain, is well posed when the spatial domain is extended to the unphysical domain $|\zeta| \geq 1$ in contrast to calculation in the physical domain $|\zeta| \leq 1$. In particular, we present evidence to suggest that there exists solution $z(\zeta, t)$ with branch point singularities behavior of a power type, i.e. $z_\zeta \sim B_0 (\zeta - \zeta_s(t))^{-\beta}$ (β non integral) as $\zeta \rightarrow \zeta_s(t)$. The form of the singularity remains invariant in time though its strength B_0 changes. A singularity does not impinge the physical domain in finite time when $\beta \geq \frac{1}{2}$.

If B denote a nondimensional surface tension, analytical evidence indicates that for $0 < B \ll 1$ for $t \ll \frac{1}{B}$, surface tension modifies the singularity structure only locally for certain kinds of singularities; yet at each initial zero of z_ζ for initial conditions independent of B , new singularities in the higher order terms of the outer asymptotic expansion in powers of B are born in $O(B^{2/7})$ time that move towards the physical domain. The singularities are smoothed out over an inner scale depending on B ; yet as they approach the physical domain, they can correspond to irregular features in a length scale larger than a surface tension dependent scale but smaller than a global scale like the channel width.

Dando, Andrew, and Sharon O. Seddougui: *The inviscid compressible Görtler problem*. ICASE Report No. 91-54, July 18, 1991, 40 pages. To be submitted to IMA Journal of Applied Mathematics.

In this paper we investigate the growth rates of Görtler vortices in a compressible flow in the inviscid limit of large Görtler number. Numerical solutions are obtained for $O(1)$ wavenumbers. The further limits of (i) large Mach number and (ii) large wavenumber with

0(1) Mach number are considered. We show that two different types of disturbance modes can appear in this problem. The first is a wall layer mode, so named as it has its eigenfunctions trapped in a thin layer near the wall. The other mode we investigate is confined to a thin layer away from the wall and termed a trapped layer mode for large wavenumbers and an adjustment layer mode for large Mach numbers, since then this mode has its eigenfunctions concentrated in the temperature adjustment layer. We are able to investigate the near crossing of the modes which occurs in each of the limits mentioned.

Nicol, David M.: *Rectilinear partitioning of irregular data parallel computations*. ICASE Report No. 91-55, July 12, 1991, 29 pages. Submitted to Journal of Parallel and Distributed Computing.

This paper describes new mapping algorithms for domain-oriented data-parallel computations, where the workload is distributed irregularly throughout the domain, but exhibits localized communications patterns. We consider the problem of partitioning the domain for parallel processing in such a way that the workload on the most heavily loaded processor is minimized, subject to the constraint that the partition be perfectly rectilinear. Rectilinear partitions are useful on architectures that have a fast local mesh network and a relatively slower global network; these partitions heuristically attempt to maximize the fraction of communication carried by the local network. This paper provides an improved algorithm for finding the optimal partition in one dimension, new algorithms for partitioning in two dimensions, and shows that optimal partitioning in three dimensions is NP-complete. We discuss our application of these algorithms to real problems.

Swanson, R. C., E. Turkel, and J. A. White: *An effective multigrid method for high-speed flows*. ICASE Report No. 91-56, July 15, 1991, 27 pages. Submitted to Journal of Communications in Applied Numerical Methods.

We consider the use of a multigrid method with central differencing to solve the Navier-Stokes equations for high-speed flows. The time-dependent form of the equations is integrated with a Runge-Kutta scheme accelerated by local time stepping and variable coefficient implicit residual smoothing. Of particular importance are the details of the numerical dissipation formulation, especially the switch between the second and fourth difference terms. Solutions are given for the two-dimensional laminar flow over a circular cylinder and a 15 degree compression ramp.

Turkel, E., R. C. Swanson, V. N. Vatsa, and J. A. White: *Multigrid for hypersonic viscous two- and three-dimensional flows*. ICASE Report No. 91-57, July 15, 1991, 23 pages. Proceedings of the AIAA 10th Computational Fluid Dynamics Conference, Honolulu, Hawaii, June 24-27, 1991, pp. 501-517.

We consider the use of a multigrid method with central differencing to solve the Navier-Stokes equations for hypersonic flows. The time-dependent form of the equations is integrated with an explicit Runge-Kutta scheme accelerated by local time stepping and implicit residual smoothing. Variable coefficients are developed for the implicit process that remove

the diffusion limit on the time step, producing significant improvement in convergence. A numerical dissipation formulation that provides good shock-capturing capability for hypersonic flows is presented. This formulation is shown to be a crucial aspect of the multigrid method. Solutions are given for two-dimensional viscous flow over a NACA 0012 airfoil and three-dimensional viscous flow over a blunt biconic.

Speziale, Charles G., and Peter S. Bernard: *The energy decay in self-preserving isotropic turbulence revisited*. ICASE Report No. 91-58, July 17, 1991, 43 pages. To be submitted to the Journal of Fluid Mechanics.

The assumption of self-preservation allows for an analytical determination of the energy decay in isotropic turbulence. Batchelor (1948), who was the first to carry out a detailed study of this problem, based his analysis on the assumption that the Loitsianskii integral is a dynamic invariant — a widely accepted hypothesis that was later discovered to be invalid. Nonetheless, it appears that the self-preserving isotropic decay problem has never been reinvestigated in depth subsequent to this earlier work. In the present paper such an analysis is carried out, yielding a much more complete picture of self-preserving isotropic turbulence. It is proven rigorously that complete self-preserving isotropic turbulence admits two general types of asymptotic solutions: one where the turbulent kinetic energy $K \sim t^{-1}$ and one where $K \sim t^{-\alpha}$ with an exponent $\alpha > 1$ that is determined explicitly by the initial conditions. By a fixed point analysis and numerical integration of the exact one-point equations, it is demonstrated that the $K \sim t^{-1}$ power law decay is the asymptotically consistent high-Reynolds-number solution; the $K \sim t^{-\alpha}$ decay law is only achieved in the limit as $t \rightarrow \infty$ and the turbulence Reynolds number vanishes. Arguments are provided which indicate that a $K \sim t^{-1}$ power law decay is the asymptotic state toward which a complete self-preserving isotropic turbulence is driven at high Reynolds numbers in order to resolve the imbalance between vortex stretching and viscous diffusion. Unlike in previous studies, the asymptotic approach to a self-preserving state is investigated which uncovers some surprising results.

Amitai, Dganit, Amir Averbuch, Samuel Itzikowitz, and Eli Turkel: *Asynchronous and corrected-asynchronous numerical solutions of parabolic PDEs on MIMD multiprocessors*. ICASE Report No. 91-59, July 17, 1991, 23 pages. Submitted to SIAM Journal on Scientific and Statistical Computing.

A major problem in achieving significant speed-up on parallel machines is the overhead involved with synchronizing the concurrent processes. Removing the synchronization constraint has the potential of speeding up the computation. We present asynchronous (AS) and corrected-asynchronous (CA) finite difference schemes for the multi-dimensional heat equation. Although our discussion concentrates on the Euler scheme for the solution of the heat equation, it has the potential of being extended to other schemes and other parabolic PDEs. These schemes are analyzed and implemented on the shared-memory multi-user Sequant Balance machine. Numerical results for one and two dimensional problems are presented. It is shown experimentally that synchronization penalty can be about 50% of run time: in most cases, the asynchronous scheme runs twice as fast as the parallel synchronous scheme. In general, the efficiency of the parallel schemes increases with processor load, with the time-level, and with the problem dimension. The efficiency of the AS may reach 90% and over, but it provides accurate results only for steady-state values. The CA, on the other

hand, is less efficient but provides more accurate results for intermediate (non steady-state) values.

Jacobs, P.A.: *Simulation of transient flow in a shock tunnel and a high Mach number nozzle*. ICASE Report No. 91-60, July 18, 1991, 15 pages. To be presented at the 4th Int. Symposium on Computational Fluid Dynamics, Davis, CA, September 1991.

A finite-volume Navier-Stokes code was used to simulate the shock-reflection and nozzle starting processes in an axisymmetric shock tube and a high Mach number nozzle. The simulated nozzle starting processes were found to match the classical quasi-one-dimensional theory and some features of the experimental measurements. The shock-reflection simulation illustrated a new mechanism for the driver-gas contamination of the stagnated test gas.

Thangam, S.: *Analysis of two-equation turbulence models for recirculating flows*. ICASE Report No. 91-61, July 19, 1991, 22 pages. Submitted to Journal of Fluids Engineering.

The two-equation $K - \varepsilon$ model is used to analyze turbulent separated flow past a backward-facing step. It is shown that if the model constants are modified to be consistent with the accepted energy decay rate for isotropic turbulence, the dominant features of the flow field – namely – the size of the separation bubble and the streamwise component of the mean velocity, can be accurately predicted. In addition, except in the vicinity of the step, very good predictions for the turbulent shear stress, the wall pressure and the wall shear stress are obtained. The model is also shown to provide good predictions for the turbulence intensity in the region downstream of the reattachment point. Estimated long-time growth rates for the turbulent kinetic energy and dissipation rate of homogeneous shear flow are utilized to develop an optimal set of constants for the two equation $K - \varepsilon$ model. The physical implications of the model performance are also discussed.

Nessyahu, Haim, and Eitan Tadmor: *The convergence rate of approximate solutions for nonlinear scalar conservation laws*. ICASE Report No. 91-62, July 24, 1991, 21 pages. Submitted to SIAM Journal on Numerical Analysis.

Let $\{v^\varepsilon(x, t)\}_{\varepsilon>0}$ be a family of approximate solutions for the nonlinear scalar conservation law $u_t + f_x(u) = 0$ with C_0^1 -initial data. Assume that $\{v^\varepsilon(x, t)\}$ are *Lip⁺-stable* in the sense that they satisfy Oleinik's E-entropy condition. We prove that if these approximate solutions are *Lip'-consistent*, i.e., if $\|v^\varepsilon(\cdot, 0) - u(\cdot, 0)\|_{Lip'(x)} + \|v_t^\varepsilon + f_x(v^\varepsilon)\|_{Lip'(x,t)} = \mathcal{O}(\varepsilon)$, then they converge to the entropy solution and the convergence rate estimate, $\|v^\varepsilon(\cdot, t) - u(\cdot, t)\|_{Lip'(x)} = \mathcal{O}(\varepsilon)$, holds. Consequently, sharp L^p and pointwise error estimates are derived.

We demonstrate these convergence rate results in the context of entropy satisfying finite-difference and Glimm's schemes.

Seddougui, Sharon O., and Andrew P. Bassom: *Nonlinear instability of hypersonic flow past a wedge*. ICASE Report No. 91-63, July 25, 1991, 42 pages. To be submitted to Journal of Theoretical and Computational Fluid Dynamics.

The nonlinear stability of a compressible flow past a wedge is investigated in the hypersonic limit. The analysis follows the ideas of a weakly nonlinear approach as first detailed by Smith (1979). Interest is focussed on Tollmien-Schlichting waves governed by a triple deck structure and it is found that the attached shock can profoundly affect the stability characteristics of the flow. In particular, it is shown that nonlinearity tends to have a stabilising influence. The nonlinear evolution of the Tollmien-Schlichting mode is described in a number of asymptotic limits which were first identified by Cowley and Hall (1990) in their linearised account of the current problem.

Duck, Peter W., Gordon Erlebacher, and M. Yousuff Hussaini: *On the linear stability of compressible plane Couette flow*. ICASE Report No. 91-64, July 29, 1991, 52 pages. Submitted to Journal of Fluid Mechanics.

The linear stability of compressible plane Couette flow is investigated. The correct and proper basic velocity and temperature distributions are perturbed by a small amplitude normal mode disturbance. The full small amplitude disturbance equations are solved numerically at finite Reynolds numbers, and the inviscid limit of these equations is then investigated in some detail. It is found that instability can occur, although the stability characteristics of the flow are quite different from unbounded flows. The effects of viscosity are also calculated, asymptotically, and shown to have a stabilizing role in all the cases investigated. Exceptional regimes to the problem occur when the wavespeed of the disturbances approaches the velocity of either of the walls, and these regimes are also analyzed in some detail. Finally, the effect of imposing radiation-type boundary conditions on the upper (moving) wall (in place of impermeability) is investigated, and shown to yield results common to both bounded and unbounded flows.

Yakhot, V., S. Thangam, T.B. Gatski, S.A. Orszag, and C.G. Speziale: *Development of turbulence models for shear flows by a double expansion technique*. ICASE Report No. 91-65, July 29, 1991, 26 pages. Submitted to Physics of Fluids A.

Turbulence models are developed by supplementing the renormalization group (RNG) approach of Yakhot & Orszag with scale expansions for the Reynolds stress and production of dissipation terms. The additional expansion parameter ($\eta \equiv S\bar{K}/\bar{\epsilon}$) is the ratio of the turbulent to mean strain time scale. While low-order expansions appear to provide an adequate description for the Reynolds stress, no finite truncation of the expansion for the production of dissipation term in powers of η suffices - terms of all orders must be retained. Based on these ideas, a new two-equation model and Reynolds stress transport model are developed for turbulent shear flows. The models are tested for homogeneous shear flow and flow over a backward facing step. Comparisons between the model predictions and experimental data are excellent.

Vatsa, Veer N., Eli Turkel, and J. S. Abolhassani: *Extension of multigrid methodology to supersonic/hypersonic 3-D viscous flows*. ICASE Report No. 91-66, August 2, 1991, 24 pages. Submitted to International Journal of Numerical Methods in Fluid Mechanics.

A multigrid acceleration technique developed for solving the three-dimensional Navier-Stokes equations for subsonic/transonic flows has been extended to supersonic/hypersonic flows. An explicit multistage Runge-Kutta type of time-stepping scheme is used as the basic algorithm in conjunction with the multigrid scheme. Solutions have been obtained for a blunt conical frustum at Mach 6 to demonstrate the applicability of the multigrid scheme to high-speed flows. Computations have also been performed for a generic High-Speed Civil Transport configuration designed to cruise at Mach 3. These solutions demonstrate both the efficiency and accuracy of the present scheme for computing high-speed viscous flows over configurations of practical interest.

Ou, Yuh-Roung: *Control of oscillatory forces on a circular cylinder by rotation*. ICASE Report No. 91-67, August 15, 1991, 17 pages. To appear in Proceedings of 4th International Symposium on Computational Fluid Dynamics... Davis, CA, September 1991.

The temporal development of forces acting on a rotating cylinder is investigated numerically in response to a variety of time-dependent rotation rates. Solutions are presented for several types of rotation that illustrate significant effects of the rotation rate on lift, drag and lift/drag coefficients. Of special interest is the formulation of an optimal control problem for the case of constant speed of rotation. We find an optimal rotation rate that achieves the maximum value of time-averaged lift/drag ratio.

Geer, James F., and Carl M. Andersen: *Resonant frequency calculations using a hybrid perturbation-Galerkin technique*. ICASE Report No. 91-68, September 11, 1991, 36 pages. To appear in Journal of Applied Mechanics.

A two step hybrid perturbation-Galerkin technique is applied to the problem of determining the resonant frequencies of one- or several-degree(s)-of-freedom nonlinear systems involving a parameter. In step one, the Lindstedt-Poincaré method is used to determine perturbation solutions which are formally valid about one or more special values of the parameter (e.g. for small or large values of the parameter). In step two, a subset of the perturbation coordinate functions determined in step one is used in a Galerkin type approximation. The technique is illustrated for several one-degree-of-freedom systems, including the Duffing and van der Pol oscillators, as well as for the compound pendulum. For all of the examples considered, it is shown that the frequencies obtained by the hybrid technique using only a few terms from the perturbation solutions are significantly more accurate than the perturbation results on which they are based, and they compare very well with frequencies obtained by purely numerical methods.

Macaraeg, Michéle G., T. L. Jackson and M. Y. Hussaini: *Ignition and structure of a laminar diffusion flame in the field of a vortex*. ICASE Report No. 91-69, September 30, 1991, 35 pages. Submitted to Combustion Science of Technology.

The distortion of flames in flows with vortical motion is examined via asymptotic analysis and numerical simulation. The model consists of a constant-density, one-step, irreversible Arrhenius reaction between initially unmixed species occupying adjacent half-planes which are then allowed to mix and react in the presence of a vortex. The evolution in time of the temperature and mass-fraction fields is followed. Emphasis is placed on the ignition time and location as a function of vortex Reynolds number and initial temperature differences of the reacting species. The study brings out the influence of the vortex on the chemical reaction. In all phases, good agreement is observed between asymptotic analysis and the full numerical solution of the model equations.

Naik, Naomi H., and John Van Rosendale: *The improved robustness of multigrid elliptic solvers based on multiple semicoarsened grids*. ICASE Report No. 91-70, September 6, 1991, 18 pages. Submitted to SIAM Journal of Numerical Analysis.

Multigrid convergence rates degenerate on problems with stretched grids or anisotropic operators, unless one uses line or plane relaxation. For three dimensional problems, only plane relaxation suffices, in general. While line and plane relaxation algorithms are efficient on sequential machines, they are quite awkward and inefficient on parallel machines. This paper presents a new multigrid algorithm, based on the use of multiple coarse grids, that eliminates the need for line or plane relaxation in anisotropic problems. We develop this algorithm, and extend the standard multigrid theory to establish rapid convergence for this class of algorithms. The new algorithm uses only point relaxation, allowing easy and efficient parallel implementation, yet achieves robustness and convergence rates comparable to line and plane relaxation multigrid algorithms.

The algorithm described here is a variant of Mulder's multigrid algorithm [5] for hyperbolic problems. The latter uses multiple coarse grids to achieve robustness, but is unsuitable for elliptic problems, since its V-cycle convergence rate goes to one as the number of levels increases. The new algorithm combines the contributions from the multiple coarse grids via a local "switch," based on the strength of the discrete operator in each coordinate direction. This improvement allows us to show that the V-cycle convergence rate is uniformly bounded away from one, on model anisotropic problems. Moreover, the new algorithm can be combined with the idea of concurrent iteration on all multigrid levels to yield a highly parallel algorithm for strongly anisotropic problems.

Carpenter, Mark H., David Gottlieb, and Saul Abarbanel: *The stability of numerical boundary treatments for compact high-order finite-difference schemes*. ICASE Report No. 91-71, September 10, 1991, 57 pages. To be submitted to Journal of Computational Physics.

The stability characteristics of various compact fourth- and sixth-order spatial operators are assessed using the theory of Gustafsson, Kreiss and Sundstrom (G-K-S) for the semi-discrete Initial Boundary Value Problem (IBVP). These results are then generalized to the fully discrete case using a recently developed theory of Kreiss. In all cases, favorable comparisons are obtained between G-K-S theory, eigenvalue determination, and numerical

simulation. The conventional definition of stability is then sharpened to include only those spatial discretizations that are asymptotically stable (bounded, Left Half-Plane eigenvalues). It is shown that many of the higher-order schemes which are G-K-S stable are not asymptotically stable. A series of compact fourth- and sixth-order schemes, which are both asymptotically and G-K-S stable for the scalar case, are then developed.

Chapman, Barbara, Piyush Mehrotra, and Hans Zima: *Vienna fortran – A fortran language extension for distributed memory multiprocessors*. ICASE Report No. 91-72, September 10, 1991, 29 pages. To appear in book "Languages, Compilers and Runtime Environments for Distributed Memory Machines", Edited by J. Saltz and P. Mehrotra, Elsevier Press.

Exploiting the performance potential of distributed memory machines requires a careful distribution of data across the processors. Vienna Fortran is a language extension of Fortran which provides the user with a wide range of facilities for such mapping of data structures. However, programs in Vienna Fortran are written using global data references. Thus, the user has the advantages of a shared memory programming paradigm while explicitly controlling the placement of data. In this paper, we present the basic features of Vienna Fortran along with a set of examples illustrating the use of these features.

Das, Raja, Ravi Ponnusami, Joel Saltz and Dimitri Mavriplis: *Distributed memory compiler methods for irregular problems – Data copying reuse and runtime partitioning*. ICASE Report No. 91-73, September 17, 1991, 35 pages. To appear in book "Languages, Compilers and Runtime Environments for Distributed Memory Machines", Editors: J. Saltz and P. Mehrotra, Elsevier Press.

This paper outlines two methods which we believe will play an important role in any distributed memory compiler able to handle sparse and unstructured problems. We describe how to link runtime partitioners to distributed memory compilers. In our scheme, programmers can *implicitly* specify how data and loop iterations are to be distributed between processors. This insulates users from having to deal explicitly with potentially complex algorithms that carry out work and data partitioning.

We also describe a viable mechanism for tracking and reusing copies of off-processor data. In many programs, several loops access the same off-processor memory locations. As long as it can be verified that the values assigned to off-processor memory locations remain unmodified, we show that we can effectively reuse stored off-processor data. We present experimental data from a 3-D unstructured Euler solver run on an iPSC/860 to demonstrate the usefulness of our methods.

Otto, S.R.: *Stability of the flow around a cylinder: The spin-up problem*. ICASE Report No. 91-74, September 17, 1991, 25 pages. Submitted to Theoretical and Computational Fluid Dynamics.

Our concern is with the flow around an infinite cylinder, which at a certain instant is impulsively started to spin. The growth of vortices in the resulting boundary layer occurring outside the cylinder is investigated. This layer is essentially a Rayleigh layer which grows

with time, so the mechanism involved is similar to that studied in Hall (1983). Vortices with wavenumber comparable to the layer thickness are shown to be described by partial differential equations. It is found necessary to solve the unsteady partial differential equations that govern the system numerically. We assume that the Rayleigh layer is thin so particles are confined to move in a path with radius of curvature the same as the cylinder. The Görtler number is a function of time, so we consider the time scale which produces an order one Görtler number. We consider the right hand branch calculation by letting the time tend to infinity, also inviscid Görtler modes are considered.

Jacobs, P.A.: *An approximate Riemann solver for hypervelocity flows*. ICASE Report No. 91-75, September 23, 1991, 15 pages. Submitted as "Technical Notes" to the AIAA Journal.

We describe an approximate Riemann solver for the computation of hypervelocity flows in which there are strong shocks and viscous interactions. The scheme has three stages, the first of which computes the intermediate states assuming isentropic waves. A second stage, based on the strong shock relations, may then be invoked if the pressure jump across either wave is large. The third stage interpolates the interface state from the two initial states and the intermediate states. The solver is used as part of a finite-volume code and is demonstrated on two test cases. The first is a high Mach number flow over a sphere while the second is a flow over a slender cone with an adiabatic boundary layer. In both cases the solver performs well.

Harten, Ami, and Sukumar R. Chakravarthy: *Multi-dimensional ENO schemes for general geometries*. ICASE Report No. 91-76, September 20, 1991, 70 pages. To be submitted to JCP.

In this paper we present a class of ENO schemes for the numerical solution of multidimensional hyperbolic systems of conservation laws in structured and unstructured grids. This is a class of shock-capturing schemes which are designed to compute cell-averages to high-order of accuracy. The ENO scheme is composed of a piecewise-polynomial reconstruction of the solution from its given cell-averages, approximate evolution of the resulting initial-value problem, and averaging of this approximate solution over each cell. The reconstruction algorithm is based on an adaptive selection of stencil for each cell so as to avoid spurious oscillations near discontinuities while achieving high order of accuracy away from them.

Harten, Ami: *Multi-resolution analysis for ENO schemes*. ICASE Report No. 91-77, September 26, 1991, 16 pages. To appear in Proceedings of the ICASE/LaRC workshop on Algorithmic Trends in CFD for the 90's.

Given a function $u(x)$ which is represented by its cell-averages in cells which are formed by some unstructured grid, we show how to decompose the function into various scales of variation. This is done by considering a set of nested grids in which the given grid is the finest, and identifying in each locality the coarsest grid in the set from which $u(x)$ can be recovered to a prescribed accuracy.

We apply this multi-resolution analysis to ENO schemes in order to reduce the number of numerical flux computations which is needed in order to advance the solution by one time-step. This is accomplished by decomposing the numerical solution at the beginning of each time-step into levels of resolution, and performing the computation in each locality at the appropriate coarser grid. We present an efficient algorithm for implementing this program in the one-dimensional case; this algorithm can be extended to the multi-dimensional case with cartesian grids.

ICASE INTERIM REPORTS

Das, Subhendu, Joel Saltz, and Harry Berryman: *A manual for PARTI runtime primitives* - Revision 1., Interim Report No. 17, April 26, 1991, 53 pages.

Primitives are presented that are designed to help users efficiently program irregular problems (e.g. unstructured mesh sweeps, sparse matrix codes, adaptive mesh partial differential equations solvers) on distributed memory machines. These primitives are also designed for use in compilers for distributed memory multiprocessors. Communications patterns are captured at runtime, and the appropriate send and receive messages are automatically generated.

Jacobs, P. A.: *Single-block Navier-Stokes integrator.*, Interim Report No. 18, July 12, 1991, 71 pages.

This report describes a program for the time-integration of the Navier-Stokes equations on a two-dimensional structured mesh. The flow geometry may be either planar or axisymmetric. The unusual features of this program are that it is written in C and makes extensive use of sophisticated data structures to encapsulate the data. The idea of writing the code this way is to make it easier (than traditional FORTRAN codes) to "parallelize" for the Multiple-Instruction-Multiple-Data style of parallel computer.

The integral form of the governing equations are given for cartesian coordinates and then the particular discretization used in the code is described. A derivation of the axisymmetric equations is given in an appendix. The full version of the code describes a flow domain as a set of abutting blocks, each consisting of a *tensor-product* mesh of quadrilateral cells. However, this report considers only the single-block version of the code. The flow field is recorded as cell-average values at cell centres and explicit time stepping is used to update conserved quantities. MUSCL-type interpolation and a three-stage Riemann solver are used to calculate inviscid fluxes across cell faces while central differences (via the divergence theorem) are used to calculate the viscous fluxes. The Riemann solver is suitable for flows with very strong shocks and does not require the entropy fix as applied to the Roe-type solvers. Because the code is intended to be a test-bed for implementation on parallel computers, the coding details are described in some detail.

A set of test problems is also included. These exercise various parts of the code and should be useful for both validation and performance measurements of the (future) parallel implementations.

Perkins, A. Louise, and Jeffrey S. Scroggs: *Proceedings for the ICASE workshop on heterogeneous boundary conditions.*, Interim Report No. 19, August 15, 1991, 78 pages.

Domain Decomposition is a complex problem with many interesting aspects. The choice of decomposition can be made based on many different criteria, and the choice of interface of internal boundary conditions are numerous. Even more interesting from a modeling perspective is that the various regions under study may have different dynamical balances, indicating that different physical processes are dominating the flow in those regions. It may

be desirable to use different numerical approximations in the regions where the physical processes are dominated by different balances.

The Institute for Computer Applications in Science and Engineering (ICASE), recognizing the need to more clearly define the nature of these complex problems, sponsored this workshop on Heterogeneous Boundary Conditions at the NASA Langley Research Center in Hampton, Virginia. This proceedings is an informal collection of the presentations and discussion groups. It also includes a bibliography that contains many of the references that discuss related topics.

The proceedings begins with summaries of the discussion groups. Then papers describing the talks are presented. Lastly, the bibliography is included, and an index by subject is provided.

ICASE COLLOQUIA

April 1, 1991 - September 30, 1991

Name/Affiliation/Title	Date
Padma Raghavan, The Pennsylvania State University "Distributed Sparse Matrix Factorization: QR and Cholesky Decompositions"	April 8
Marten T. Landahl, Massachusetts Institute of Technology "Algebraic Instability and the Near-Wall Reynolds Stresses"	April 9
Hans P. Zima, University of Vienna, Austria "Compiling for Distributed-Memory Machines: Experiences and Recent Research"	April 15
Ricardo D. Pantazis, Duke University "Parallel Solution of the Symmetric Generalized Eigenvalue Problem"	April 16
Francois Irigoin, Centre de Recherche en Informatique, France "Automatic Interprocedural Parallelization"	April 19
Suresh Chittor, Michigan State University "Communication Performance of Multicomputers"	April 19
Alan Sussman, Carnegie-Mellon University "Model-Driven Mapping onto a Distributed Memory Parallel Computer"	May 2
Michael Gerndt, University of Vienna "Compiling Sequential Programs for Shared-Memory and Distributed-Memory Multiprocessors"	May 3
Jacques Periaux, Dassault Aviation, France "Finite Element Simulations of Hypersonic Reacting Flows: Numerical Tools for the Design of the European Hermes Space Vehicle"	May 9
Hermann F. Fasel, The University of Arizona, Tucson "Numerical Simulation of Laminar-Turbulent Transition in Shear Flows"	May 15

Name/Affiliation/Title	Date
Steven Zenith, Ecole Nationale Supérieure des Mines de Paris, France "Process Interaction Models: A Brief Description of and Rationale for Ease"	May 16
Matthew Rosing, University of Colorado, Boulder "Language Support for Numerical Programs on Distributed Memory Multiprocessors"	May 17
William T. Ashurst, Sandia National Laboratories "Geometry of Premixed Flames in Three-Dimensional Turbulence"	May 17
Fabio Bertolotti, Princeton University "Investigations of Laminar-Turbulent Transition in Subsonic and Supersonic Boundary Layers Using the Parabolic Stability Equations"	May 22
Asok Ray, The Pennsylvania State University "Damage-Mitigating Control of Aerospace Structures for High Performance and Extended Life"	June 4
Rajesh Aggarwal, Columbia University "Parallel Algorithms in Computational Mechanics"	June 14
J. Peraire, Imperial College of Science and Medicine, London "The Computation of Three Dimensional Flows Using Unstructured Meshes"	June 19
Carl Scarbnick, Scientific Computing Associates "Algorithms for Solving Problems in Scientific Computation"	June 24
Lawrence Crawl, University of Rochester "Architectural Adaptability in Parallel Programming"	June 28
Jean Paul Boujot, CISI Ingenierie, France "Will Computer Architectures be Specified by Numerical Methods?"	July 15
I. G. Angus, Northrop Research and Technology Center "Parallelism, Object Oriented Programming Methods, Portable Software and C++ (A CFD Example)"	July 16

Name/Affiliation/Title	Date
Mark Jones, Argonne National Laboratory "An Efficient Parallel Iterative Solver for Large Sparse Linear Systems"	July 18
Ishfaq Ahmad, Syracuse University "Dynamic Task Scheduling and Load Balancing for Large Multicomputer Systems"	July 19
Isaac Harari, Stanford University "Finite Element Methods for the Reduced Wave Equation: Design and Analysis"	July 22
Robert Krasny, University of Michigan "Vortex Sheet Computations: Roll-Up, Wakes, Separation"	August 1
John Crepeau, University of Utah "Dynamical Systems Study of Mixing and Boundary Layers"	August 9
Daniel Joseph, University of Minnesota "Finite Size and Nonlinear Effects in Fluidized Suspensions"	August 13
M. Karpel, Technion - Israel Institute of Technology, Haifa, Israel "Multidisciplinary Optimization of Aeroservoelastic Systems Using Reduced-Size Models"	August 15
James Antaki, University of Pittsburgh "The Artificial Heart: Prospective Need for CFD"	August 26
Charles Fineman, NASA Ames Research Center "AIMS: A Software Visualization Tool"	August 28
Philip Rosenau, Technion, Haifa, Israel "On Mathematical Modeling of High Gradient Phenomena"	August 29
Rolf Radespiel, DLR, Braunschweig, Germany "Progress with Multigrid Schemes for Hypersonic Flow Problems"	September 5
Robert Weaver, University of Colorado "Supporting Dynamic Data Structures at the Language Level on Distributed Memory Machines"	September 10

Name/Affiliation/Title	Date
V. Venkatakrishnan, Computer Sciences Corporation and NASA Ames Research Center "A MIMD Implementation of a Parallel Euler Solver for Unstructured Grids"	September 19
Ami Harten, Tel Aviv University and ICASE "Multi-Dimensional Essentially Non-Oscillatory (ENO) Schemes for General Geometries"	September 20
David Mount, University of Maryland "Computational Geometry and Mesh Generation"	September 20

ICASE SUMMER ACTIVITIES

The summer program for 1991 included the following visitors:

<u>NAME/AFFILIATION</u>	<u>DATE OF VISIT</u>	<u>AREA OF INTEREST</u>
Saul S. Abarbanel Tel-Aviv University, Israel	6/24 - 8/30	Computational Fluid Dynamics
Remi Abgrall INRIA	7/1 - 8/30	Computational Fluid Dynamics on Unstructured Meshes
H. Thomas Banks University of Southern California	6/3 - 6/14	Control Theory
Alvin Bayliss Northwestern University	6/10 - 6/13	Numerical Solution of PDE's
Scott Beryman Yale University	5/20 - 8/30	Software for Parallel Systems
Shahid Bokhari Pakistan University of Engineering and Technology	7/8 - 9/6	Parallel Computing Systems
John A. Burns VPI and State University	6/10-14	Control Theory
Claudio Canuto Politecnico di Torino, Italy	9/10-20	Spectral Methods for PDE's
Barbara Chapman University of Vienna	8/14-28	Compiler Development for Multiprocessors
Craig Chase Cornell University	5/20 - 8/30	Distributed Memory Architectures
William Criminale University of Washington	8/26 - 9/6	Transition and Turbulence
Wai-Sun Don Brown University	6/10 - 7/26	Computational Fluid Dynamics

<u>NAME/AFFILIATION</u>	<u>DATE OF VISIT</u>	<u>AREA OF INTEREST</u>
Peter L. Duck University of Manchester, England	7/8 - 9/20	Computational Fluid Dynamics
Dennis Gannon Indiana University, Bloomington	8/5-9	Parallel Programming Environments
James Geer State University of New York	9/19-23	Asymptotic Methods for Differential Equations
Ann Gelb Brown University	6/17-28	Numerical Analysis
David Gottlieb Brown University	6/17 - 8/16	Numerical Methods for PDE's
Satyanarayan Gupta Old Dominion University	6/3 - 8/12	Unstructured Mesh Calculations for the Connection Machine
Philip Hall University of Manchester, England	6/24 - 8/2 9/25-10/18	Computational Fluid Dynamics
Amiram Harten Tel-Aviv University	9/1-27	Numerical Methods for PDE's
Daniel J. Inman State University of New York, Buffalo	6/3-14	Numerical Methods for Inverse Problems in Distributed Systems
Kazufumi Ito University of California, Los Angeles	6/3-7	Control Theory
Ashwani Kapila Rensselaer Polytechnic Institute	8/5-16	Mathematical Aspects of Combustion Processes
Mordechay Karpel Technion-IIT, Haifa, Israel	7/8 - 9/6	Modeling of Aeroservoelastic Systems
David R. Keyes Yale University	8/12-30	Parallel Numerical Procedures Combustion
Fumio Kojima Osaka Institute of Technology, Japan	8/5-30	Probabilistic and Stochastic Methods for Optimal Control Problems

<u>NAME/AFFILIATION</u>	<u>DATE OF VISIT</u>	<u>AREA OF INTEREST</u>
Robert Krasny University of Michigan	7/29 - 8/2	Vortex Methods and Vortex Dynamics
Marten Landahl Massachusetts Institute of Technology	8/26-30	Transition and Turbulence
Jacques Liandrat I.M.S.T., France	6/10-14	Numerical Algorithms for Nonlinear PDE
Robert MacCormack Stanford University	7/29 - 8/2	Numerical Methods for the Solution of the Equations of Fluid Mechanics
Moshe Matalon Northwestern University	6/3-14	Hydrodynamic Instability in Chemically Reacting Flows
K. W. Morton Oxford University	9/13-21	Computational Fluid Dynamics
H. S. Mukunda Indian Institute of Science, Bangalore	5/29 - 6/21	High Speed Reacting Flows
Naomi H. Naik Vassar College	8/5-30	Multigrid Methods
David Nicol College of William and Mary	5/13-17 8/16-22	Techniques for Mapping Algorithms onto Parallel Systems
D. Papageorgiou New Jersey Institute of Technology	5/20-31	Computational Fluid Dynamics
Terry Pratt University of Virginia	5/21-24 6/11-14 6/18-21 8/5-9 8/26-30	Characteristics of Languages for Parallel Computers
Rolf Radespiel DLR, Institute for Design Aerodynamics	6/17 - 9/14	Numerical Methods for High Speed Flows
Asok Ray The Pennsylvania State University	5/20 - 6/7	Control Systems for Flexible Space Structures

<u>NAME/AFFILIATION</u>	<u>DATE OF VISIT</u>	<u>AREA OF INTEREST</u>
Philip Roe The University of Michigan	8/5-23	Computational Fluid Dynamics
Jeffrey Scroggs North Carolina State University	5/10 & 17 8/5-16	Domain Decomposition Techniques for Partial Differential Equations
Chi-Wang Shu Brown University	6/3 - 7/5	Computational Fluid Dynamics
Alex Solomonoff Brown University	6/13-28	Numerical Methods for PDE's
Eitan Tadmor Tel-Aviv University	7/8 - 8/2	Numerical Solution of Partial Differential Equations
Saleh Tanveer Ohio State University	6/17-28 9/9-13	Modelling of Crystal Growth
Hein Tran North Carolina State University	6/3-7	Control Theory
Eli Turkel Tel-Aviv University	6/24 - 8/23	Computational Fluid Dynamics
Bram van Leer University of Michigan, Ann Arbor	8/12-13 9/16-20	Computational Fluid Dynamics
Sesh Venugopal Rutgers University	5/20 - 8/16	Partitioning of Scientific Problems on Parallel Computers
Eric Voth Brown University	6/24 - 7/8	Computational Fluid Dynamics
Claus Wagner University of Florida	6/10 - 7/6	Problems of Instabilities in Incompressible Flows
Yun Wang University of Southern California	6/10-14	Mini Mast Models for Identification and Control
Hans Zima University of Vienna	8/14-28	Compiler Development for Multiprocessors

OTHER ACTIVITIES

The Transition and Turbulence Workshop co-sponsored by ICASE and NASA Langley Research Center was held July 8 - August 2, 1991, at NASA Langley Research Center. Over one hundred people attended this workshop. The objective was to encourage development and validation of Reynolds-averaged two-equation and second-order closure models as well as subgrid scale models for the transitional and fully turbulent zone. A volume of the proceedings from this conference will be published by Springer-Verlag in the near future.

On September 15-17, 1991 a Workshop on Algorithmic Trends in CFD for the 90's co-sponsored by ICASE and NASA Langley Research Center was held at the Holiday Inn-Hampton-Coliseum Hotel and Conference Center. One hundred and ten people attended this workshop. The purpose of the workshop was to bring together numerical analysts and computational fluid dynamicists i) to assess the state of the art in the areas of numerical analysis particularly relevant to CFD, ii) to identify promising new developments in various areas of numerical analysis that will have impact on CFD, and iii) to establish a long-term prospective focussing on opportunities and needs.

A volume of the proceedings from this workshop will be published by Springer-Verlag in the near future.

ICASE STAFF

I. ADMINISTRATIVE

Robert G. Voigt, Director Ph.D., Mathematics, University of Maryland, 1969. Numerical Algorithms for Parallel Computers

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Holly D. Joplin, Office Assistant (Part-time)

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Shelly D. Millen, Technical Publications Secretary

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Emily N. Todd, Executive Secretary/Visitor Coordinator

II. SCIENCE COUNCIL for APPLIED MATHEMATICS and COMPUTER SCIENCE

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Joseph Olinger, Professor, Computer Science Department, Stanford University.

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Stanley J. Osher, Professor, Mathematics Department, University of California.

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Gordon Erlebacher - Ph.D., Plasma Physics, Columbia University, 1983. Computational Fluid Dynamics. (November 1989 to November 1994)

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VI. SCIENTIFIC STAFF

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Peter W. Protzel - Ph.D., Electrical Engineering, Technical University of Braunschweig, Germany, 1987. Reliability of Computing Systems. (March 1987 to September 1991)

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Ralph C. Smith - Ph.D., Numerical Analysis, Montana State University, 1990. Theoretical and Computational Issues Associated with Inverse Problems. (August 1990 to August 1993)

Alan Sussman - Ph.D., Computer Science, Carnegie-Mellon University, 1991. Quantifying and Predicting Performance of Realistic Applications on Distributed Memory Parallel Computers. (August 1991 to August 1993)

VII. VISITING SCIENTISTS

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